Climate Science for a Sustainable Energy Future (CSSEF)

Project Start Date: October 1, 2010
Project End Date: September 30, 2015

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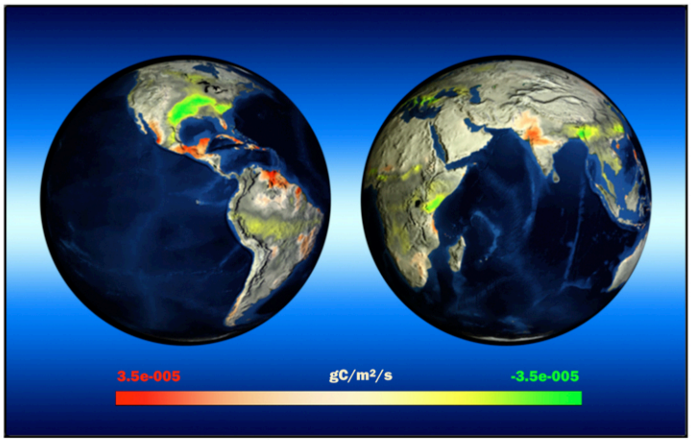
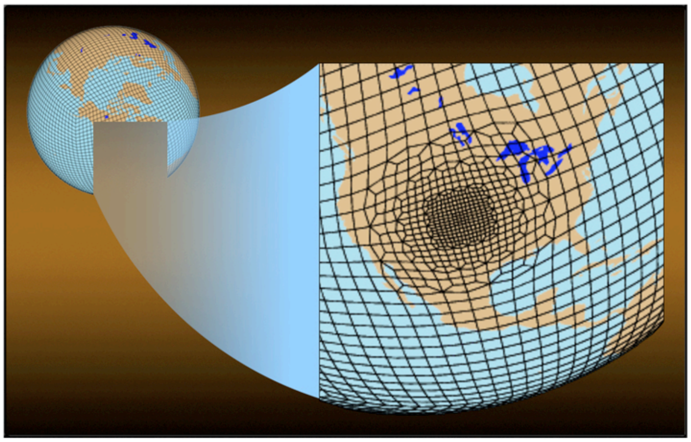
Oak Ridge National Laboratory
Principal Investigator: David C. Bader

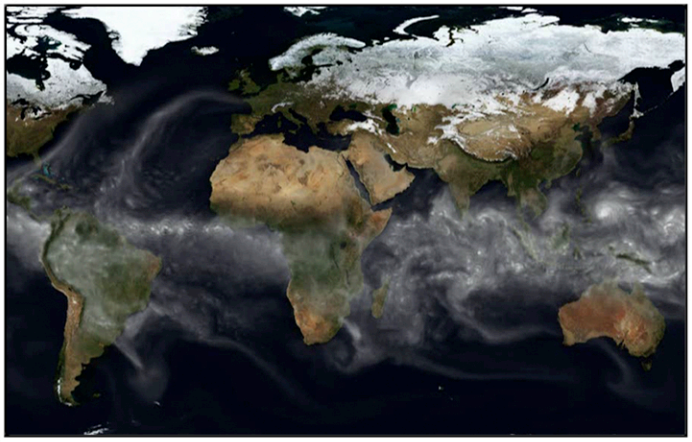
Contributing Organizations

Argonne National Laboratory
Brookhaven National Laboratory
Lawrence Berkeley National Laboratory
Lawrence Livermore National Laboratory
Los Alamos National Laboratory
National Center for Atmospheric Research
Pacific Northwest National Laboratory
Sandia National Laboratories

U.S. Department of Energy
Office of Science
Office of Biological and Environmental Research







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Cover Page

Climate Science for a Sustainable Energy Future

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Funding Period: October 1, 2010, through September 30, 2015

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Dean N. Williams	Software Project Leader	Lawrence Livermore National Laboratory

Requested Funding

By year					Total
2011	**2012**	**2013**	**2014**	**2015**	
16,001,964	16,001,962	16,001,960	16,001,973	16,001,937	80,009,796

Use of human subjects: NO
Use of vertebrate animals: NO

CONTENTS

BUDGETS

BUDGET AND BUDGET EXPLANATION

ORNL will serve as the lead laboratory for the CSSEF project, and thus all funds will flow through ORNL to the CSSEF laboratories. The following is a budget breakdown by laboratory by fiscal year.

	2011	2012	2013	2014	2015	Total
ORNL	$4,239,654	$4,239,652	$4,239,650	$4,239,663	$4,239,627	**$21,198,246**
ANL	$1,659,000	$1,659,000	$1,659,000	$1,659,000	$1,659,000	**$8,295,000**
BNL	$331,800	$331,800	$331,800	$331,800	$331,800	**$1,659,000**
LANL	$2,322,600	$2,322,600	$2,322,600	$2,322,600	$2,322,600	**$11,613,000**
LBNL	$1,659,000	$1,659,000	$1,659,000	$1,659,000	$1,659,000	**$8,295,000**
LLNL	$1,957,620	$1,957,620	$1,957,620	$1,957,620	$1,957,620	**$9,788,100**
PNNL	$1,858,080	$1,858,080	$1,858,080	$1,858,080	$1,858,080	**$9,290,400**
SNL	$1,974,210	$1,974,210	$1,974,210	$1,974,210	$1,974,210	**$9,871,050**
TOTALS	**$16,001,964**	**$16,001,962**	**$16,001,960**	**$16,001,973**	**$16,001,937**	**$80,009,796**

The ORNL totals include a subcontract for services from NCAR. The following is a breakdown of the proposed annual (unburdened) subcontract totals.

	2011	2012	2013	2014	2015	Total
NCAR	$872,820	$849,541	$891,623	$911,438	$944,255	$4,469,677

Following this introduction are budget pages and justifications for all CSSEF partners. This information is presented beginning with ORNL (which includes the NCAR detailed budget sheet and justification), followed by the remaining laboratories in alphabetical order. Each of the CSSEF laboratories has provided a letter of commitment at the beginning of their budget section.

Per the Guidance Document (Appendix 1), we approximately meet the funding levels specified. The funding levels were broken out as follows in the Guidance:

a) Converting observational data sets into specialized, multi-variable data sets for model testing and improvement ($3M)
b) Development of model development testbeds in which model components and sub-models can be rapidly prototyped and evaluated ($3M)
c) Research to enhance numerical methods and computational science research focused on enabling climate models that use future computing architectures ($4M)
d) Research to enhance efforts in uncertainty quantification for climate model simulations and predictions ($5M)
e) Project management ($1M)

The CSSEF team combined the data and testbed items into a single crosscutting area (data/testbed). The table shown on the next page provides a detailed breakdown of the science funding levels targets, including the distribution across the research themes. The resulting funding levels were as follows:

- $5.7M for data/testbed (vs. $6M for the combined areas),
- $3.65M for numerical methods and computational science (vs. $4M), and
- $4.65M for UQ (vs. $5M).

The difference of ~$900,000 annually is for the NCAR subcontract as this is not included in the numbers in the following table.

ABSTRACT

Proposal for the Climate Science for a Sustainable Energy Future Project
By Oak Ridge National Laboratory
David C. Bader, Principal Investigator
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The Climate Science for a Sustainable Energy Future (CSSEF) is a collaborative project among Oak Ridge, Argonne, Brookhaven, Lawrence Berkeley, Lawrence Livermore, Pacific Northwest, and Sandia national laboratories together with the National Center for Atmospheric Research to transform the climate model development and testing process and thereby accelerate the development of the Community Earth System Model's sixth-generation version, CESM3, scheduled to be released for predictive simulation in the 5 to 10 year time frame. Four research themes are addressed in the project: (1) a focused effort for converting observational data sets into specialized, multi- variable data sets for model testing and improvement, (2) development of model development testbeds in which model components and sub-models can be rapidly prototyped and evaluated, (3) research to enhance numerical methods and computational science research focused on enabling climate models that use future computing architectures, and (4) research to enhance efforts in uncertainty quantification for climate model simulations and predictions.

These four themes are mutually reinforcing and tightly coupled around three overarching research directions: (1) the development, implementation, and testing of variable-resolution methodologies that enable computationally efficient simulation of the climate system at regional scales, (2) improvement of the representation of the hydrological cycle and quantification of the sources of certainty in its simulation, and (3) the reduction and quantification of uncertainties in carbon cycle and other biogeochemical feedbacks in the terrestrial ecosystem. The CSSEF will be structured to first deploy expertise in the research theme areas across the development of the atmosphere, ocean, sea ice, and land surface model components, and later to the fully coupled system.

The CSSEF project addresses the DOE Office of Biological and Environmental Research's Long-Term Measure to ***"Deliver improved scientific data and models about the potential response of the Earth's climate and terrestrial biosphere to increased greenhouse gas levels for policy makers to determine safe levels of greenhouse gases in the atmosphere."***

I. INTRODUCTION

Climate simulation and prediction have entered a new and more-demanding era with the recognition that global temperatures are increasing and will continue to increase at an accelerating rate from the accumulation of greenhouse gases (GHGs) in the atmosphere. The Intergovernmental Panel of Climate Change (IPCC) Fourth Assessment Report (IPCC, 2007) documented that global climate models could reproduce historical global warming trends and provide insight into future climate change that will result from the continued accumulation of atmospheric GHGs. Nevertheless, global models lack the fidelity to accurately predict with quantified uncertainty how climate will change on regional scales and how that change will emerge in the next few decades, information that would specifically benefit the nation and the U.S. Department of Energy (DOE). Equally important, better and more accurate Earth system simulation will help inform near-term energy policy choices that have long-term (decades to century) implications. Developing the scientific and computational capacity to produce these predictions will require transformative rather than evolutionary change in climate simulation as it enters the era of seamless prediction across broad time and space scales (Hurrell et al. 2009).

As documented in *Advancing the Science of Climate Change* (U.S. NRC 2010) the information required from climate change predictions extend beyond the questions posed by the IPCC in the upcoming Fifth Assessment Report (IPCC 2010), scheduled for release in 2013. Within its mission, DOE desires to understand the future interactions between climate change and energy security with greater quantitative detail and accuracy than is possible now. Consequently, the DOE Office of Science issued guidance to its national laboratories to collectively develop a proposal for the Climate Science for a Sustainable Energy Future (CSSEF) project to bring the tremendous scientific assets in its laboratory system to meet the ongoing and long-term challenges in advancing climate prediction (Appendix 1). The guidance states that the CSSEF "…will address a critical and relatively straightforward objective—to accelerate the incorporation of new knowledge, including process data and observations, into climate models and to develop new methods for rapid validation of improved models. A crosscutting objective of CSSEF is to develop novel approaches to exploit computing at the level of many tens of petaflops in climate models. These challenges are recognized broadly in the climate community, and DOE is well equipped to address them.

Climate model development is a mature and ongoing enterprise that has numerous and diverse participants, ranging from graduate students in academic programs to senior leaders in dedicated climate research laboratories. The CSSEF will have its maximum impact through integration with the core long-term development of the Community Earth System Model (CESM) project. The CESM, formerly the Community Climate System Model, is a long-standing collaborative and internationally recognized effort that has involved the National Center for Atmospheric Research (NCAR), several DOE national laboratories and numerous academic institutions for over 15 years. The collaboration has produced four generations of State-of-the-Science global climate models, including the most recent, CESM1. While much of the community effort is now dedicated to application of CESM1 and the development of CESM2, CSSEF will focus on the long-term development of CESM3, which is consistent with plans described in the *CESM Science Plan* (Appendix 2). The paradigm of multiple, parallel development paths to build successive generations of predictive models explicitly acknowledges that aspects of model development, particularly those requiring significant new research tasks, take longer time between model releases. While aspects of development require 10 to 15 years, a new major new version of CESM is released every 5 to 6 years.

CSSEF will undertake several unique and potentially transformative research directions, including

- The capability to thoroughly test and understand the uncertainties in the overall model and its components as they are being developed;
- Major scientific advances in the components that will achieve greater fidelity in modeling feedbacks in the climate system;
- Development of model evaluation procedures that allow the rapid ingest of observational data for model and component evaluation;
- Flexible dynamical cores that enable fine-scale simulations; and
- Early adaptation of the model algorithms and code to the next generation of computers.

The combination of unique research capabilities in the DOE laboratory system and a focus on long-term development has the potential to realize a transformed CESM enterprise that will serve as a truly national resource.

II. APPROACH

The Climate Science for a Sustainable Energy Future (CSSEF) project's objective is to transform the climate model development and testing process and thereby accelerate the development of the Community Earth System Model's (CESM's) sixth-generation version, CESM3 (generations 1, 2, and 3 were labeled CCSM1 to CCSM3). This model has been informally designated as the "next plus one," and "current plus two" version of CESM, but here we describe it simply as CESM3. In addition, at the end of 5 years this project will construct a unified scientific, computational, and empirical foundation for CESM4. This foundation is critical to ensure that the CESM4 community can fully exploit the unprecedented technological advancements anticipated toward the end of the decade, including extreme-scale computing platforms and the Decadal Survey space-based observational platforms and instruments (http://science.nasa.gov/earth-science/decadal-surveys/).

Figure II.1 provides a conceptual schematic of the complete development and application enterprise required to construct, integrate, test, and deploy climate models as complex and comprehensive as CESM. In this view, model development and application occur simultaneously. Furthermore, simulation results continue to be analyzed and used by scientific communities for several years after the completion of the model runs. The philosophy behind CSSEF is based on the understanding that many aspects of model development and evaluation, from early research through full implementation and testing, take 10 to 15 years to accomplish, while new versions of climate models are released at approximately 5 to 6 year intervals for predictions, projections, and applications.

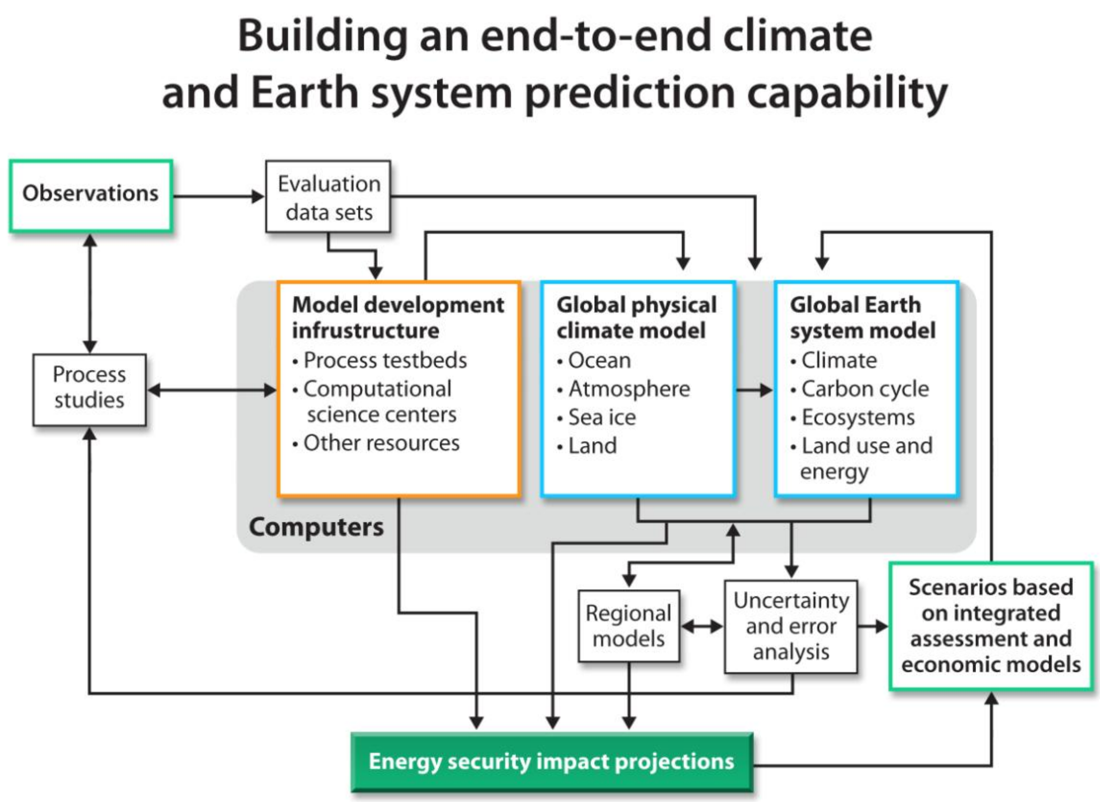

Fig. II.1. Conceptual view of an ongoing climate simulation and prediction enterprise such as the CESM project. New versions of models are developed from increased understanding gained through the integration of observations, process research and earlier model studies.

Existing models are deployed on high end computing resources to produce simulations and predictions of climate for analysis and applications.

DOE explicitly identified four research themes in its guidance (Appendix 1) to us for the preparation of this proposal. These themes are based on core competencies and expertise within its laboratory system, which will have major, positive impacts on the long term direction of CESM. The themes are as follows

1. A focused effort for converting observational data sets into specialized, multi-variable data sets for model testing and improvement.
2. Development of model development testbeds in which model components and submodels can be rapidly prototyped and evaluated.
3. Research to enhance numerical methods and computational science research focused on enabling climate models that use future computing architectures.
4. Research to enhance efforts in uncertainty quantification for climate model simulations and predictions.

In our CSSEF project proposal, these four themes are mutually reinforcing and tightly coupled. Figure II.2 displays the straightforward relationships among them. For example, uncertainty quantification methodologies require observational data and model testbeds to compare models to observations. Additionally, numerical methods have intrinsic errors and uncertainties that non-linearly propagate through the model system and require quantification. Consequently, the CSSEF project takes an integrative, rather than a reductionist, approach to employing these capabilities to advance climate prediction.

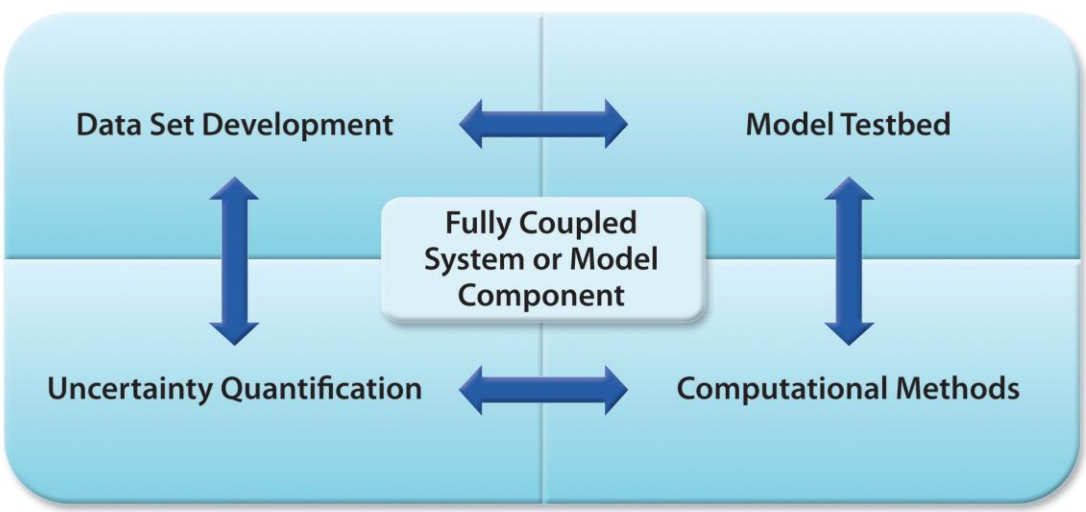

Fig. II.2 Relationships among the four research themes.

We take a comprehensive view of the improvements required in improving model accuracy and reducing uncertainty. The CSSEF project has three overarching and intersecting directions, all of which are highlighted as high-priority needs in *Advancing the Science of Climate Change* (NRC 2010). First, we will develop, implement and test variable resolution methodologies, which enable computationally efficient simulation of the climate system at regional scales. Second, we will employ CSSEF capabilities to improve the representation of the hydrological cycle and quantify the sources of uncertainty in its simulation. Third, we anticipate making significant progress in reducing and quantifying uncertainties in carbon cycle and other biogeochemical feedbacks in the terrestrial ecosystem. These directions require consideration of the fully coupled system and are reflected in the long-term project milestones. Somewhat opposing our ambition to be integrative, however, long-term model research proceeds within the sub-model component framework. To keep a holistic view, the CSSEF will be structured to deploy laboratory expertise in the research theme areas across the development of the model components (Fig. II.3). As will be seen in the following chapters, each of the major model components will exploit the research themes in a manner tailored to their needs.

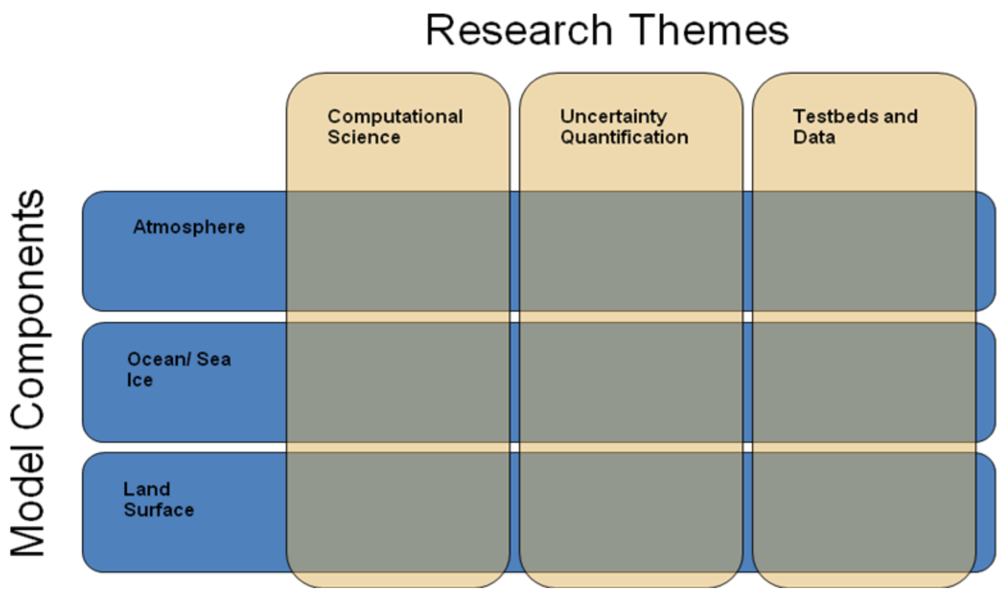

Fig. II.3. CSSEF project structure.

We strongly emphasize that this effort is not the complete picture of CESM3 development. CSSEF results and products will be integrated with other community research activities as part of the CESM enterprise. To guarantee that happens, NCAR scientists and CESM leadership are full partners with the DOE laboratories in the CSSEF, which will fund dedicated scientists at NCAR to work with the component working group co-chairs and liaisons to integrate CSSEF results into CESM. In addition, we will fully adhere to both the formal policies and informal culture of free and open exchange that have been hallmarks of the CESM program since its inception.

In the following chapters, we present a more detailed vision for the CSSEF. Chapter III provides background on the motivation for the project. Chapters IV, V, and VI describe plans for advancing the CESM3 model components through the employment of the research theme capabilities. Chapters VII, VIII, and IX address crosscutting activities along the research theme areas. The remaining chapters describe the organizational model for the project, its deliverables and its relationship to other research activities.

III. BACKGROUND

The CSSEF project continues DOE's internationally recognized leadership role in advancing climate simulation and prediction. In collaboration with the National Science Foundation, DOE established at NCAR an early modeling program to simulate greenhouse gas warming (Washington and Meehl 1984). DOE pioneered the development of model intercomparison studies and coordinated large-scale international climate simulation experiments when it established the Program for Climate Model Diagnosis and Intercomparison (PCMDI) in 1989 (Cess et al. 1989, Gates 1992). The DOE Computer Hardware, Advanced Mathematics and Model Physics (CHAMMP) program was the international leader in developing climate models that were able to efficiently exploit a new generation of distributed-memory, massively parallel computer architectures. (Dukowicz et al. 1993, Drake 1995, Washington et al. 2000). Because of these forward thinking investments many computational aspects of the Community Earth System Model (CESM) and its predecessors have relied heavily on the expertise at DOE laboratories (Drake 2005). Shortcomings in climate models' representation of clouds led DOE to launch the Atmospheric Radiation Measurement (ARM) Program (Ackerman and Stokes 2003, Stokes and Schwartz 1994) to close critical understanding gaps with additional observations. The need to more tightly incorporate these new observations in the model development process led to an an early prototype for the CSSEF testbeds. This effort was described by Phillips, et al. (2004) and Klein et al. (2006), who directly employed ARM data to test climate model cloud parameterizations. Randerson et al. (2009) describe a DOE-supported terrestrial carbon-cycle model intercomparison project that proposes a standardized testbed for future studies.

III.1 MOTIVATION FOR DATA AND TESTBED RESEARCH

Building on this history, the CSSEF bridges two areas of research identified in the DOE Climate Change Research Program: Strategic Plan, (http://www.sc.doe.gov/ober/Climate%20Strategic%20Plan.pdf), Climate Change Process Research, which is focused on "resolving the most critical uncertainties underlying projections of climate change," and Climate Change Modeling, with a focus on, "advancing the computer models needed to understand climate change and its consequences." CSSEF will have an impact on two of the three Grand Challenges (decadal climate prediction and Earth system simulation) identified by the DOE Biological and Environmental Research Advisory Committee (BERAC 2008) to guide long-term directions in DOE's climate research program. That report specifically recommended a research initiative to "(Incorporate) knowledge gained from observational and modeling process studies into multiple generations of Earth System models."

III.2 MOTIVATION FOR NUMERICAL METHODS AND COMPUTATIONAL SCIENCE RESEARCH

Several recent reports (WCRP 2008, ASCAC/BERAC 2008 and BERAC 2009) have stressed the need for the climate modeling community to undertake research programs to address the numerical, computational, and computer science aspects of climate and Earth system simulation on future generations of high-performance scientific supercomputers. Within its national laboratory system, DOE supports world-leading expertise in these areas as well as the computational facilities on which climate simulation and prediction are conducted. The CSSEF will leverage this expertise and these facilities to lead the community as it undergoes the transition to a new generation of computer architectures in much the same way as the CHAMMP program did during the last architectural transition.

III.3 MOTIVATION FOR UNCERTAINTY QUANTIFICATION RESEARCH

As documented in the above referenced reports, climate change prediction is one of the most complex problems undertaken by the scientific simulation community. Quantifying and even reducing the uncertainty of future climate predictions and projections continues to be one of the highest priority research issues. In recent years, formal methods of verification, validation, and uncertainty quantification (UQ) employed in other simulation problems have been applied to climate simulation (e.g., Stainforth et al. 2005, Murphy et al. 2007, Murphy et al. 2009, Jackson et al. 2008). In the UQ community, verification refers to gathering evidence that the models and simulations are mathematically accurate, validation refers to investigating whether the models are physically accurate, and UQ refers to quantifying the impact of all sources of uncertainty on the model predictions. All of these activities are referred to as UQ within this proposal. Besides the enormous complexity in the physics and the scarcity of observations, UQ in climate simulations is particularly challenging due to the requirement of extrapolation, in this case to predict future events. Fortunately, this situation is analogous to the challenges faced by other security-oriented communities grounded in the physical sciences and supported by DOE (LLNL 2004). Those communities have a successful record of managing extrapolations from observations using a combination of computer modeling and UQ analysis. An appreciable fraction of the UQ expertise in the proposed CSSEF project is leveraged from those other communities.

IV. ATMOSPHERIC MODEL DEVELOPMENT

IV.1. SCIENCE GOALS

How water moves through the atmosphere is a central issue in climate science with enormous implications for society as well as the carbon cycle. Furthermore, the poor simulation of the water cycle by today's atmospheric models is a large impediment to the development of policy-relevant predictions for climate change mitigation and adaptation. The organizing goal of CSSEF atmospheric model development is the creation of a weather-resolving global atmosphere model that better simulates the water cycle.

To achieve this goal, we envision the following central components:

- An atmospheric testbed that uses in situ and satellite water cycle observations to rapidly calibrate the model in a systematic and reproducible way using techniques developed by the uncertainty quantification (UQ) community
- Computational science research to facilitate the running of weather-resolving atmospheric models on Leadership Computing Facility (LCF) computational resources and the development of models capable of mesh refinement and nonhydrostatic dynamics
- Focused parameterization development as needed to address the fact that the target resolution of the model is approaching the regime where nonhydrostatic dynamics become important

By the end of this 5 year project, we will produce a global atmosphere model with about 10 km horizontal resolution with integration rates suitable for multi-century climate modeling and a companion testbed that can be used to further improve the model. We will also be in the early stages of producing a model with statically refined resolutions as fine as 3 km that would be suitable for shorter-term process studies and comparison to a more sophisticated nonhydrostatic adaptive mesh refinement dynamical core under development (see Chapter VII). We envision that the 10 km global atmosphere model—a so-called "weather-resolving climate model"—will become a formal released configuration of the Community Atmosphere Model (CAM) and be suitable for global climate integrations as part of the Community Earth System Model (CESM).

Given the number of efforts worldwide that seek to develop global "cloud resolving" models (i.e., models with 1 km resolution) (Miura et al. 2007a), one might ask, is our focus on the development of a model with 10 km too conservative? We emphatically believe that our goal is the appropriate goal for the climate modeling community today and will yield significant benefits for climate prediction for a number of reasons. First, even with aggressive exploitation of evolving LCF resources, integration rates of global cloud-resolving models will remain too slow to support multi-century integrations needed for climate, much less tuning integrations necessary to develop a high-quality model. In contrast, it will be feasible within 10 years to perform multi-century integrations of a global model with 10 km resolution. Second, 10 km is about the finest resolution for which a model with hydrostatic dynamics and long-time step physical parameterizations can credibly be configured for the purposes of climate simulations. It is more straightforward to modify today's climate models for this configuration than it is to convert limited area cloud-resolving models into a global climate models. Third, as ocean models are moving to the eddy-resolving domain with resolutions of 10 km, simulated air-sea interactions (Xie 2004) will benefit from having the atmosphere and ocean at comparable resolutions. This is in contrast to today's situation, where many climate models have horizontal resolution much finer in the ocean than in the atmosphere. Finally, a 10 km model begins to provide the regional climate change impact information needed by policy makers.

With the water cycle as the primary science driver, we aim to improve the representation of a number of specific phenomena, including (1) the frequency and intensity of tropical cyclones, (2) the probability distribution function of rainfall intensity, (3) the dominance of summertime nocturnal propagating convective systems over the central United States, (4) tropical intraseasonal variability, (5) the frequency of drizzle in stratiform boundary layer clouds, and (6) the regional balance between local evaporation and precipitation. Based on scientific reasoning and work elsewhere involving tropical cyclones (Zhao et al. 2009, Bender et al. 2010) and intraseasonal variability (Miura et al. 2007b), we expect that the resolution of mesoscale processes by a 10 km model permits, but does not guarantee, a successful simulation of many of these phenomena. We thus believe that creating a well-tuned atmospheric model with 10 km resolution will be an important step toward accomplishing the goal of delivering credible climate predictions of the water cycle from a global physical model.

The remainder of this chapter presents our plans for an atmospheric testbed and the data used therein (Section IV.2), computational science and numerical methods research (Section IV.3), and the use of uncertainty quantification techniques in the atmospheric testbed (Section IV.4).

IV.2. TESTBEDS AND DATA

Testbed Requirements. Development of this next-generation atmospheric climate model requires the creation of a new testbed, although we will leverage data sets and technique development where appropriate from the existing DOE atmospheric testbeds (Phillips et al. 2004, Fast et al. 2010, Liu et al. 2010). Our requirements include (1) quantifiable model-observation comparison techniques embedded with systematic and reproducible optimization of perturbed physical parameters, (2) utilization of the latest water cycle observations from ground-based and satellite instruments, (3) testing of the three-dimensional (3D) climate model, and (4) computational efficiency to permit parameter optimization of high-resolution simulations.

Testbed Design. The atmospheric testbed (Figure IV.1 and Table IV.1) consists of two components: a calibration platform and a validation platform. The calibration platform is where UQ techniques are used to calibrate the model against local data sets, such as those provided by the Atmospheric Radiation Measurement (ARM) (Ackerman and Stokes 2003) Climate Research Facility sites (ACRF) at a number of fixed sites. In contrast, the validation platform is where independent global observations are used to demonstrate the impact of calibration to the local data sets on the fidelity of the global climate simulation.

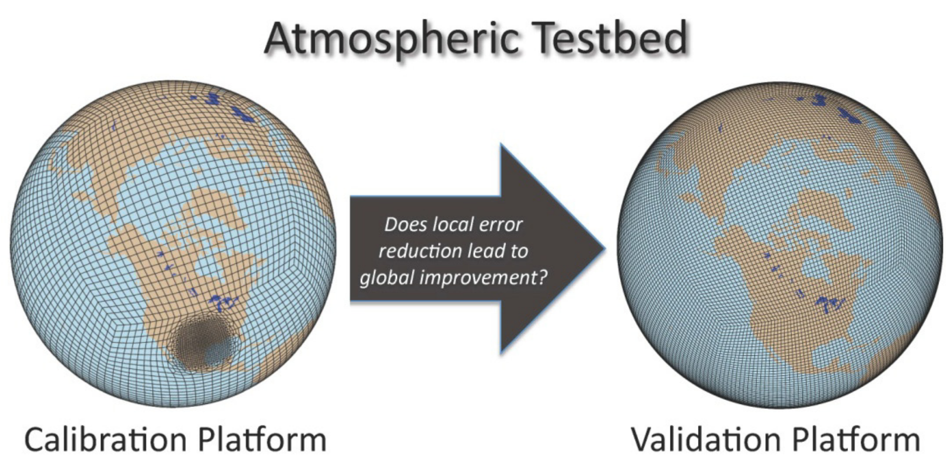

Figure IV.1. Schematic of the Atmospheric Testbed. For display purposes, grid sizes differ from those of Table IV.1.

Table IV.1. Characteristics of Calibration and Validation Platforms

	Calibration Platform	Validation Platform
Model Construction	Global model with static mesh refinement above sites of interest	Global model with uniform grid
Forcing	Weather-forecast mode with nudging to analysis data on coarse outer grid	Free-running climate mode with initial condition from analysis data
Initial Resolution	1/8° fine mesh transitioning to 1°	1/8° everywhere
Uncertainty Quantification Methods	Parameter tuning: calibration of uncertain parameters with local data sets	Ensemble of simulations with parameter sets generated by parameter tuning
Data sets	Local water cycle data sets such as ACRF site data	Global data sets such as satellite or re-analysis data

Calibration Platform. The calibration platform is the central component of the testbed. It is where the model will be calibrated to local scale observational data from ACRF sites using uncertainty quantification techniques. In order to efficiently compare many model versions with local observations, we will utilize the stretched grid capability of dynamical cores to provide regional resolution refinement over sites of interest.

Section IV.3 provides further details of the proposed model grid and the development of dynamical cores that support variable resolution, including multiple regions (such as ACRF sites) with fine resolution in a single integration. To facilitate comparison to the local data sets, we will perform integrations in weather-forecast mode by nudging the atmosphere-state fields to global re-analyses. Nudging strength will decay in amplitude as one approaches the region of interest where the model will be allowed to run freely. Consistent with trying to improve the parameterized physics given a large-scale state of the atmosphere, the influence on the global domain from processes simulated over the finest portion of the mesh will be heavily damped.

The ability to have a fine mesh over a region of interest facilitates extensive use of ground-based ACRF data sets. In particular, we will focus on ACRF sites where deep convection is common such as the central United States Southern Great Plains site (SGP) in summer and three sites (Darwin, Manus, and Nauru) in the tropical western Pacific. We will also use data from the ACRF mobile facility campaign to the Azores in 2009–2010 to measure marine stratocumulus clouds. While the ACRF has historically focused on observations of cloud and radiation processes, the program has recently added a new focus in precipitation supported by new instruments funded by the 2009 American Reinvestment and Recovery Act. Currently, the program is installing new scanning precipitation (and cloud) radars at all its sites that will help address the water cycle questions of interest to this project.

Validation Platform. The second component of the atmospheric testbed is the validation platform, which will test the hypothesis that model calibration to one or more fixed-site data sets yields improved global simulations of water cycle processes. In this platform, a global model with uniform resolution is integrated in "climate mode," driven only by observed sea-surface temperatures and sea-ice distributions (Gates et al. 1992). In model development cycles, these integrations are routinely performed for ~20 years of simulated time to demonstrate the fidelity of a model's climate. Due to its computational expense, in the first years of the project, only limited ensembles of such runs are possible at the initial 1/8° global resolution. Later, we expect these integrations will become more feasible once we adapt to future-generation computer platforms. In the meantime, the validation platform will utilize shorter-duration integrations of a year or two. We note that other groups utilizing weather-resolving climate models also utilize short integrations to investigate their model's climate (Miura et al. 2007a). While these integrations are too short to validate subtle aspects, they are sufficient for identifying gross climate errors, including those involving the water cycle.

IV.2.1 Data Sets, Diagnostics, and Metrics

A central component of the testbed is quantitative evaluation with observations. As such, the quantitative evaluation must produce metrics (or skill scores) that can be used in parameter optimization.

IV.2.1.1 Calibration Platform Metrics

Metrics for the calibration platform will be tailored to advanced process-oriented observations available from ACRF instruments. Metric development involves four steps: (1) deriving geophysical quantities from raw instrument data; (2) processing data to remove bad or missing values, fill gaps, and average to appropriate time scales; (3) adding uncertainty estimates; and (4) defining quantifiable metrics that test important aspects of the water cycle and can be computed from the model.

Initial metric development will focus on data sets for which the derivation of geophysical quantities and assignment of uncertainty estimates are straightforward. Targeted development of higher-order data sets will be pursued thereafter. The initial efforts will focus on one-dimensional (1D) time series of basic quantities measured by surface instrumentation: temperature (T); relative humidity (RH); precipitation rate (PRECIP); surface radiation, hemispheric cloud fraction (CF); and precipitable water vapor (PWV); and liquid water path (LWP) under nonprecipitating conditions. We will build upon the Climate Modeling Best Estimate (CMBE) products (Xie et al. 2010), which contain data-satisfying steps 1 and 2 above by adding uncertainty estimates to the geophysical quantities, allowing flexible averaging times (to represent multiple spatial scales), and automating the processing in the testbed environment. Common procedures for gridding data, quality checks, and averaging will be implemented so that they can easily be applied to any data set. As errors in T, RH, and PRECIP are typically well characterized (Srivastava 2008, WMO 2008, Ritsche 2009), we will propagate uncertainty estimates from raw measurements through to final averaged properties. Furthermore, we will examine model PWV and LWP values only in nonprecipitating conditions for which the current instrumentation produces valid measurements. We note that new ACRF instruments should improve measurements during drizzle conditions.

For these 1D variables, we will develop metrics that assess both the magnitude and variability of the parameters, including hourly, daily, or weekly means, standard deviation, and skewness. To assess the diurnal cycle, we will examine simple metrics such as the relative magnitude of values at 6, 12, 18, and 24 coordinated universal time (UTC) to the value at 0 UTC, and more complicated metrics such as composite diurnal anomalies or semidiurnal harmonics (Dai and Trenberth 2004). We will also work with the uncertainty quantification group to develop more sophisticated methods of directly using the probability distribution information to evaluate and tune the model.

The above data sets will serve as baseline metrics for the calibration testbed, but other than surface precipitation rate, they do not specifically target the water cycle. Building on this experience, we will begin targeted development of higher-order data products that specifically address precipitation processes. These data sources (listed in Table IV.2 in order of priority) are briefly discussed below.

Higher order precipitation statistics. As marine boundary layer clouds are important for climate sensitivity (Bony and Dufresne 2005), it is important to accurately model how often these clouds drizzle under different meteorological and aerosol conditions, as this has implications for surface precipitation, cloud lifetime, and cloud radiative effects (Stevens and Feingold 2009). Using the vertically pointing radar (and scanning cloud radars when available), we will use reflectivity thresholds to identify drizzle and calculate drizzle frequency for the Azores ACRF deployment.

Table IV.2. Sample Metrics for Calibration Platform and Data Sources

Metric	Data Source
Surface T, RH, PRECIP, CF and radiation (time series, diurnal cycle, probability density functions)	Climate Modeling Best Estimate (Xie et al. 2010)
Higher-order and 2D precipitation statistics (drizzle frequency, rain area, stratiform/convective partitioning)	Scanning precipitation radars at SGP, Darwin and Manus sites
CFADs of cloud radar reflectivity and Doppler velocity to evaluate cloud vertical structure and microphysics	ACRF cloud radars + instrument simulators modified for ground-based instruments (Haynes et al. 2007; Bodas-Salcedo et al. 2008, Chepfer et al. 2008, Fan et al. 2009)
Diabatic heating (time series, diurnal cycle, lead-lag correlation of diabatic heating profile relative to surface precipitation time series)	ACRF multi-year variational analysis at SGP and Darwin, and radar-derived latent heating (Xie et al. 2004; Schumacher et al. 2004)
EIS, LTS, CAPE (Klein and Hartmann, 1993; Wood and Bretherton 2006)	ACRF radiosonde observations at all sites; Raman lidar and/or AERI retrievals at SGP and ACRF tropical sites
Relationships between variables: water vapor vs. precipitation; regime decomposition such as stratification by vertical velocity (Holloway and Neelin 2010; Bony et al. 2004)	Various ACRF measurements, reanalysis data for vertical velocity

At the other end of the intensity scale, deep convective systems produce significant amounts of precipitation and are major challenges for climate models. Current model problems include the diurnal cycle, the transition from shallow to deep convection, the relative amounts of convective and stratiform rain (Dai 2006), and an overprediction of graupel. Using the scanning precipitation radars, we will develop metrics related to classification of hydrometeors, frequency of stratiform and convective rain, and rain area (Steiner et al. 1995, May and Keenan 2005). Uncertainty estimates for rain rate from precipitation radars are well known (Ciach et al. 2007) although uncertainties for the higher order products are less clear. To add uncertainties to these quantities, we will explore sensitivities to thresholds used to define the various parameters.

We will also investigate the utility of metrics derived from multi-variable relationships, such as the relationship between column integrated water vapor and precipitation (Bretherton 2004, Holloway and Neelin 2009, 2010); the relationship between upper-tropospheric tropical water vapor and cloud-radiative forcing (Bennhold and Sherwood 2008); and time lags between precipitation and thermodynamic parameters (Mapes et al. 2006).

Cloud vertical structure and microphysics and instrument simulators. ACRF vertically pointing radars and lidars provide information on cloud vertical structure and microphysics. Quantitative comparisons of retrieved cloud properties to model simulations can be difficult for two reasons. First, radar and lidar instruments can saturate in precipitation or optically thick cloud so that upper level clouds may not be detected if lower clouds exist. Second, the retrieval of cloud microphysics from radar and lidar measurements is an under-constrained inverse problem that requires assumptions whose impacts on retrieved variables are difficult to quantify. To address these issues, scientists have developed instrument simulators which perform forward calculations to transform model variables into simulated observations that can be directly and quantitatively compared to observations (Klein and Jakob 1999, Bodas-Salcedo et al. 2008).

Performing a forward calculation rather than an under-constrained inverse problem reduces ambiguity in the model-observational comparisons through more comparable sampling of observations and model results and allows more straightforward estimation of uncertainties. Errors in the observed quantities can be determined from propagation of errors related to calibration, instrument noise, and other factors. Errors in the simulated quantities can be estimated based on forward-model sensitivity tests.

A suite of satellite simulators for climate model evaluation have been developed (Bodas-Salcedo et al. 2008) and in parallel, simulators for ground-based radar and lidar instruments have been developed for higher-resolution cloud-resolving models (Fan et al. 2009). We will modify the existing climate model simulators to simulate the ACRF ground-based radar and lidar measurements, including lidar backscatter, radar reflectivity and Doppler velocity. Inclusion of Doppler velocity could be an important constraint on ice particle fall velocities that have been shown to strongly affect climate sensitivity experiments (Sanderson et al. 2008). Metrics associated with the instrument simulators will include probability distributions of the radar reflectivity and Doppler velocity as a function of height (cloud frequency altitude diagrams (CFADs) (Yuter and Houze 1995).

Diabatic and latent heating profiles. Diabatic heating is the general driver of the atmospheric circulation. The vertical structure of diabatic heating varies significantly between different cloud and precipitation regimes (Zhang et al. 2010), so models must produce the correct frequency of precipitation regimes to produce the correct diabatic heating profiles. The multi-year constrained variational analysis technique (Zhang and Lin 1997, Xie et al. 2004) uses radiosondes, surface observations, and scanning precipitation radars to provide a consistent multi-state description of the state over the ACRF sites, including vertical profiles of diabatic heating. Some measure of the uncertainty in the diabatic heating is possible by propagating the surface precipitation rate uncertainty through the variational analysis algorithms (Christian Jakob, personal communication).

Thermodynamic vertical structure. The vertical structures of temperature, water vapor, and atmospheric stability are also important influences and constraints on cloud and precipitation processes. Observations have shown that stratiform low cloud fraction is strongly correlated with lower tropospheric stability (LTS) and the estimated inversion strength (EIS). We will use ACRF radiosonde observations to calculate metrics associated with thermodynamic vertical structure. At the SGP site, high temporal resolution profiles of temperature and humidity profiles derived from the Atmospheric Emitted Radiance Interferometer (AERI) and Raman lidar are also available and will be used to derive with higher temporal resolution similar metrics including the convective available potential energy (CAPE).

Other considerations. The metrics chosen may be sensitive to the spatial and/or temporal averaging, and may vary with dynamical regime. We will explore how optimized parameter values vary when metrics are averaged over different temporal or spatial scales. The relationship of water variables to dynamics, as exemplified by regime analysis (Bony et al. 2004, Jakob et al. 2005), provides a potent tool that permits a partial separation of errors in model physics from those in model dynamics. We will explore techniques to separate the observations into different dynamical regimes, and compare to similar regimes constructed from model output. This will allow us for a more penetrative analysis of the effect on the parameter optimization on simulated water cycle quantities.

IV.2.1.2 Validation Platform Diagnostics

For the validation platform, we will use an independent set of observations to test the improvements that result from the calibration with local data sets. We envision building on the standard CAM diagnostics package by adding diagnostics that emphasize the water cycle using data sets with global coverage. Candidate diagnostics (Table IV.3) include the geographical distribution of time mean precipitation from the Climate Prediction Center Merged Analysis of Precipitation (CMAP) and the Global Precipitation Climatology Project (GPCP), the probability distribution function of precipitation intensity including stratiform and convective partitioning and frequency of precipitation in boundary layer clouds from CloudSat and the Tropical Rainfall Measurement Mission (TRMM), the distribution, number and

Table IV.3. Sample Diagnostics of Validation Platform and Their Data Sources

Diagnostic	Data Source
Hurricane statistics	IBTrACs (Knapp et al. 2010)
Global precipitation, and tropical precipitation intensity statistics	CMAP (Xie and Arkin 1997); GPCP (Huffman et al. 1997); TRMM (Kummerow et al. 2000)
Cloud/precipitation vertical structure statistics (satellite simulator CFADs)	Calipso/CloudSat instrument simulations (Bodas-Salcedo et al. 2008)
Drizzle Incidence in boundary layer clouds	CloudSat (Berg et al. 2010)
Multi-variate relationships between water vapor, precipitation and radiative forcing	SSM/I (Peters and Neelin 2006); Reanalysis data (Wheeler and Kiladis 1999); ERBE/HIRS (Bennhold and Sherwood 2008)
Standard core diagnostics: large-scale wind, temperature, and humidity; cloud fraction; SW and LW radiation	ECMWF or other reanalysis (Kalnay et al. 1996, Uppala et al. 2005); ISCCP (Rossow and Schiffer 1991); CERES (Wielicki et al. 1996)
MJO diagnostics	MJO working group (Kim et al. 2009)

intensity of tropical cyclones (Knapp et al. 2010), the wavenumber-frequency distributions of tropical precipitation or outgoing longwave (LW) radiation (Wheeler and Kiladis 1999), the diurnal cycle of precipitation and new climatologies of water cycle components at continental and ocean basin scales from the NASA Energy and Water Cycle (NEWS) program. The observational data sets will be primarily based upon preexisting data sets, although we may need to derive specific quantities for the time periods and model resolutions.

Supplementing the water cycle diagnostics will be a small set of core diagnostics related to atmospheric dynamics, thermodynamics, cloud, and radiation fields such as the latitude-height distribution of zonal mean zonal wind, temperature, and relative humidity from re-analyses, the geographical distribution of outgoing LW and absorbed shortwave (SW) radiation from the Clouds and the Earth's Radiant Energy System satellite (CERES), global cloud cover from the International Satellite Cloud Climatology Project (ISCCP), and frequency distributions of cloud vertical structure from CloudSat. Additionally, we will include the newly developed set of Madden-Julian Oscillation (MJO) diagnostics (Kim et al. 2009).

IV.2.2 Data and Workflow Infrastructure

The operation of the atmospheric testbed will require significant support from the data infrastructure team. In particular, we envision support is necessary to automate the integrations and diagnostics of both platforms. This involves script development and standardization, diagnostic package development, accumulation and cataloging of global data sets, developing the capability to extract frequent time resolution data subsets from the fine mesh used in the calibration platform, and interaction of model integrations with an uncertainty quantification framework.

Additional necessary modifications to the existing CAM diagnostics package include customization for the water cycle diagnostics of interest and evaluation at higher spatial resolution utilizing higher resolution observations. Some of this effort can leverage work from existing DOE project, *Ultra High Resolution Global Climate Simulation to Explore and Quantify Predictive Skill for Climate Means, Variability and Extremes*, James Hack, Principal Investigator. In addition, one might desire assistance in the automation of run-time diagnostics such as the global probability distribution functions of high-resolution quantities or the on-line implementation of simulator diagnostics only for the calibration platform's fine mesh regions.

IV.2.2.1 Testbed and Data Miletones and Deliverables

Year 1

- Initial design and prototype of calibration testbed, including at least one data set and metric
- Initial design of data archiving
- Initial design for calibration data sets and metrics and validation diagnostics
- Initial design and prototype of validation platform

Years 2–3

- Working version of testbed including automation
- Robust data archiving and visualization tools for atmospheric comparisons
- Implementation of calibration data sets/metrics in testbed including in-line computation of second-order diagnostics to reduce input and output need
- Instrument simulator modified for ground-based data
- Working version of validation platform

Years 4–5

- Production version of testbed
- Robust automated procedures for analysis/visualization
- Implementation of diagnostics and metrics from new ACRF instrumentation
- Instrument simulator incorporated into model diagnostics and metrics
- Expanded global diagnostics of precipitation for validation platform

IV.3 COMPUTATIONAL SCIENCE AND NUMERICAL METHODS

IV.3.1 Dynamical Core Requirements

To be successful, we seek a global atmospheric dynamical core with the following capabilities: (a) resolutions as fine as 3 km globally, (b) scaling to very large number of processing elements, (c) successful exploitation of the new computational architectures that will be available for climate simulation, (d) static mesh refinement to permit more detailed simulation over fixed-locations such as ACRF sites, and (e) nonhydrostatic dynamics, when desired. Characteristics (a) and (b) imply the need for a non-latitude-longitude grid core of which several candidate dynamical cores exist.

Because it has many of the necessary characteristics, we will use the High-Order Method Modeling Environment (HOMME) dynamical core described below as the standard "workhorse" dynamical core for the testbed. A number of actions are necessary to convert HOMME into a dynamical core with these defined characteristics. These actions include (a) the implementation of CAM (both HOMME and the model physics) on the next generation LCFs, (b) the development of static mesh regional refinement configurations with resolutions as fine as 1/8° for the calibration platform, and (c) improvements to the data analysis and visualization work flow. Preliminary global 1/8° CAM-HOMME simulations show that the CCSM's parallel input and output capability is adequate for monthly mean data but may need improvements for high temporal resolution output. A larger bottleneck will be the analysis tool-chain, which will be required to support distributed processing of unstructured grid data. This later task is the focus of at least one recently awarded BER project, *Parallel Analysis Tools and New Visualization Techniques for Ultra-Large Climate Data Sets*, Robert Jacob, Principal Investigator.

We note that the regional refinement capabilities of HOMME will complement a parallel effort to develop the computational framework for the application of nonhydrostatic *dynamic* adaptive capabilities (see Chapter VI). This adaptive framework will exploit the atmospheric testbed and provide a basis for quantitative comparison and evaluation of a non-hydrostatic formulation across a variety of scales. It will also allow for exploration of the benefits of resolving time-dependent localized features in global-scale models.

IV.3.2 CAM-HOMME Overview

HOMME is a scalable dynamical core that is available as an option in CAM (Neale et al. 2010). HOMME introduces a new horizontal discretization in CAM based on the spectral element method which is a type of the continuous-Galerkin finite element method. The spectral element configuration used in HOMME is fourth-order accurate and designed for fully unstructured quadrilateral meshes. HOMME is the first unstructured grid dynamical core integrated into CAM. Other aspects of the dynamical core are based on a combination of other well-tested approaches, such as the vertically Lagrangian discretization of tracer advection from CAM's finite volume dynamical core (Lin 2004). The dynamics are modeled after that used by CAM's global spectral model, sharing the same vertical coordinate, vertical discretization, hyper-viscosity based horizontal diffusion and top-of-model dissipation (Neale et al. 2010). The spectral element discretization in HOMME is based on an earlier research code called the Spectral Element Atmosphere Model (SEAM). Both SEAM and HOMME have been extensively verified beginning with shallow water test cases (Taylor et al. 1997, Thomas and Loft 2002) and continuing through 3D dry dynamical test cases (Taylor et al. 1998, Thomas and Loft 2005, Dennis et al. 2005, Taylor et al. 2007, Lauritzen et al. 2010), idealized aqua planet experiments with full physics (Taylor et al. 2008, Mirsha et al. 2010) and Earth-geography simulations with CAM2 physics (Wang et al. 2007). CAM-HOMME is currently being tuned for CAM4 physics for both 1° and 1/4° resolutions as part of the DOE high-resolution project of James Hack.

HOMME brings several new capabilities to CAM. The spectral element method is *compatible*, meaning that it has discrete versions of the divergence and Stokes theorems (Taylor and Fournier 2010). This property allows HOMME to locally conserve both mass and energy, making it the first dynamical core in CAM that can run without an ad-hoc energy *fixer* (Taylor 2010). The unstructured grid capability means that CAM can use quasi-uniform grids such as those based on the cubed-sphere (Figure IV.2, left panel). This allows CAM to use full two-dimensional (2D) domain decomposition that was not possible with the older dynamical cores in CAM based on latitude-longitude grids. The 2D domain decomposition results in unmatched scalability for an atmospheric model on today's petascale platforms (Dennis et al. 2005, Taylor et al. 2008). In Figure IV.3, we show this scalability on two LCFs. At (1/4°) global resolution, CAM-HOMME has nearly perfect scalability on Intrepid, scaling out to 86,000 cores, representing one element per core. The

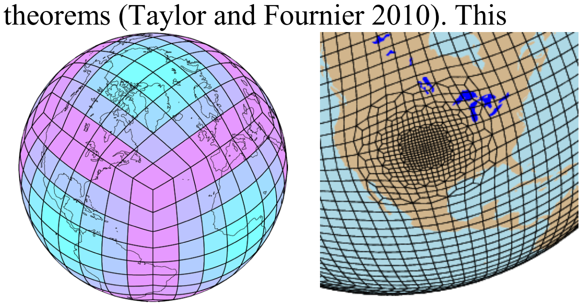

Figure IV.2. Some of the horizontal grids it is now possible to use in CAM5 when running with the HOMME dynamical core. Left: A low-resolution quasi-uniform resolution cubed-sphere grid. Right: Close-up view of a variable resolution global grid with localized mesh. refinement over the SGP ACRF site.

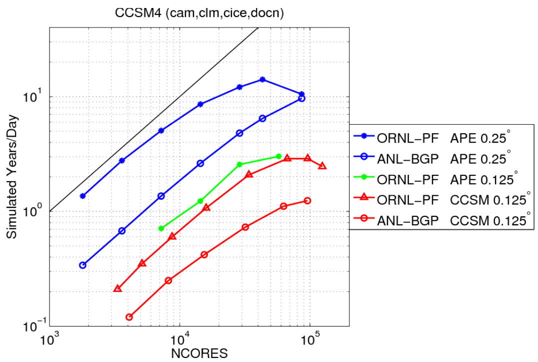

Figure IV.3. Strong scaling to 100,000 processor cores on the Jaguar-PF and Intrepid-BGP systems. CCSM denotes realistic Earth geography configurations. APE denotes idealized aqua-planets configurations.

1/8° benchmarks show the performance of the full CCSM in a standard-atmosphere-only realistic geography configuration running at 2.9 simulated years per day (SYPD). At this resolution, CAM-HOMME will support up to 350,000 message-passing interface (MPI) tasks.

IV.3.3 CAM5 Variable Resolution Development

The unstructured grid capability of CAM-HOMME makes it possible to use variable resolution grids such as shown in the right panel of Figure IV.2. The spectral element method has been designed from inception to support such grids, and all the numerical properties of the method (conservation, fourth-order accuracy) are retained on such grids. In 2D, local mesh refinement with spectral elements has been shown to be effective at reducing the global solution errors when refinement is used over dynamically significant regions such as localized topography (Fournier et al. 2004, St. Cyr et al. 2008). In realistic models, variable resolution has long been used in global forecast models, starting with Schmidt (1977) and Staniforth and Mitchell (1978) and continuing through Markovic et al. (2010). For climate modeling, the work is more recent (Fox-Rabinovitz et al. 1997, Cote et al. 1997), including a version of CAM2 with the spectral element method (Baer et al. 2006). There are now several funded and proposed DOE and National Science Foundation projects exploring variable resolution in CAM4 and CAM5 that share staff with CSSEF.

Here, we have the unique focus of using variable resolution for the calibration of our target global-high-resolution configuration of CAM-HOMME. We will first construct suitable grids with a high-resolution region over ACRF sites, with resolution matching the target for the global model. These grids will be created using CUBIT (http://cubit.sandia.gov), a successful mesh generation package that constructs conforming quadrilateral meshes using a paving algorithm (Parrish et al. 2007). CUBIT was used to construct the example grid shown in the right panel of Figure IV.2, which has an average global grid spacing of 110 km, transitioning to a region with 20 km resolution over the SGP ACRF site. It has 50X fewer elements than a global 20 km grid, representing a 50X computational savings with the potential to be increased further with multi-rate time-stepping algorithms.

For the calibration application, some experimentation must be done to determine the appropriate size of the high-resolution region, the size of the transition region between low and high-resolution, preparation of appropriate topography and surface roughness data sets and the scaling of the resolution dependent parameters in the dynamics. This can be guided by previous work using structured grids with stretching (Fox-Rabinovitz et al. 2006, Fox-Rabinovitz et al. 2008). For calibration, the more difficult issue of resolution dependent physics parameterizations is minimized, since the calibration will be against detailed measurements only in the region of high resolution. We will also introduce a multi-rate time-stepping method into CAM-HOMME so that most of the domain is not restricted to the small time-step required in the high-resolution regions.

There is a numerical issue that must be addressed when using local refinement when no constraints are placed on the large-scale dynamics. This configuration will potentially be used if calibration will occur without nudging or for obtaining improved regional climate simulations within CAM. This is consequence of the ill-posedness of the atmospheric primitive equations at open boundary conditions (Oliger and Sundström 1978, Temam and Tribbia 2003). Vertical waves removed by the hydrostatic approximation introduce a non-locality in the horizontal directions that creates numerical problems in the transition region from high to low resolution (Tribbia 2010). This issue will also have to be addressed in non-hydrostatic models, since non-hydrostatic approaches either remove the same vertical waves or severely distort them through the use of implicit time-stepping methods (Tribbia 2010). In particular, we will test the addition of a second order vertical derivative term to the primitive equations following Temam and Tribbia (2003). Further refinements, such as making this term more scale selective, will also be pursued.

Depending on the success of these efforts, we will then use the validation testbed to develop configurations of CAM with regionally refined resolution and which produce quantified improvements in regional climate statistics. The ultimate goal will be to allow regional refinement to resolutions sufficiently fine enough to allow the exploration of non-hydrostatic and cloud-resolving effects in century long CAM simulations.

IV.3.4 CAM5 Weather-Resolving Configurations

One of our key goals is the development of a global configuration of HOMME with CAM5 model physics, 1/8° horizontal resolution and increased vertical resolution. Past experience has shown that producing new scientifically validated configurations of CAM can take several years. The proposed testbed will greatly accelerate this process, but the testbed must first be given a configuration of the model that is capable of being tuned, and this will still require model development and scientific insight to diagnose possible problems. In particular, we will need to address the issues that arise in applying CAM5 physics to HOMME and in the creation of the variable-resolution HOMME. As an example, the initial simulations of CAM with the finite volume dynamical core at 1/4° resolution developed large and unstable polar jets, which had to be controlled by additional changes to the dynamics. Early results with HOMME at 1/8° resolution with CAM4 physics look promising. The model is stable and producing reasonable simulations, especially with regards to capturing increased mesoscale variability (Figure IV.4) and tropical cyclone activity (not shown).

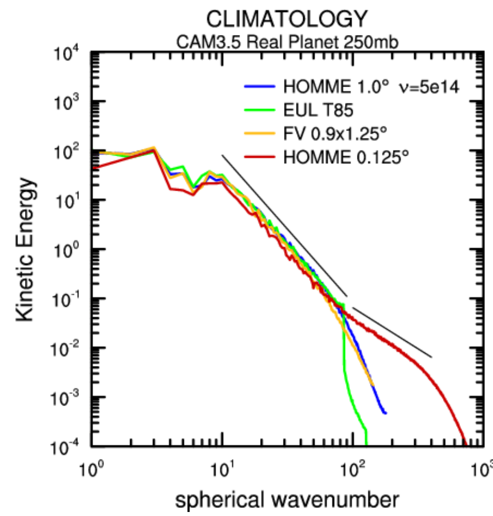

Figure IV.4. At 1/8°, CAM-HOMME fully resolves both (a) the large-scale quasi-two-dimensional enstrophy-cascade regime where the wave number k^{-3} scaling in the kinetic energy spectra is well captured by models at 1° and (b) the observed $k^{-5/3}$ mesoscale shallowing regime associated with increased variability of extreme events. The black curves show a –3 slope (upper line) and a –5/3 slope (lower black line).

IV.3.5 Performance on Next-Generation LCF

We intend to fully use of next-generation LCF systems as soon as they become available. In order to estimate the type of performance needed to achieve our goal of a global 1/8° resolution model running at 5 SYPD, we first make the reasonable assumptions that the model will use CAM5 physics, increase the vertical resolution from 30 levels to 60 levels, and reduce the physics time-step from 30 min to 10 min. Such a configuration will be 11X more expensive than the 1/8° simulation results given above. These numbers are based on the fact that the column physics will become 6X more expensive and be called 3X more often, the dynamics will not change, advection will become 8X more expensive due to the advection of more species, and the assumption that the increase in the number of vertical levels will linearly increase the total cost. For our 1/8° simulations described above, the best performance number obtained to date is 3 SYPD. To obtain 5 SYPD, we thus need an 18X increase in performance. On a next-generation LCF system, this can be obtained through only a 2X increase in scalability and a 10X increase in node performance. This is in line with expectations of these systems, which we believe will have a modest increase in the number of nodes, but each node will have a 10X increase in performance due to the introduction of more cores and or accelerators.

To achieve a 10X performance increase on these next-generation nodes, we will require a significant effort porting both the HOMME dynamical core and the CAM5 model physics. The breakdown in cost between dynamics (including advection) and model physics will be approximately 2:1, so both components are significant and must be considered. The largest cost will be tracer advection which is estimated to represent 50% of the total. It also represents the easiest target for increased performance, as the expected 25 tracers can all be advected concurrently and independently. Specifically, efforts under CSSEF will focus on direct improvements to the existing models and the model implementation changes needed to exploit the upcoming LCFs, which will likely employ hybrid computer architectures.

IV.3.6 Computational Sciences and Numerical Methods Milestones and Deliverables

Year 1

- Deliver high- and low-resolution CAM5 configurations for testbed
- Deliver CAM5 variable resolution: initial configurations with refinement to 1/8° resolution

Years 2–3

- Deliver CAM5 high-res configuration at 1/8° running efficiently on O(100,000) cores with integration rates to support decadal simulations
- Optimize configurations for the variable resolutionCAM5 with respect to refinement rate, dissipation, and time-stepping

Years 4–5

- Deliver a CAM5 high-resolution configuration at 1/8° running at 5 SYPD on both LCFs
- Fully integrate variable-resolution configurations into CAM for improved regional climate modeling

IV.4 UNCERTAINTY QUANTIFICATION IN THE ATMOSPHERIC TESTBED

The outcome of the calibration platform will be metrics that quantify agreement between model simulations and observations. These metrics can be used to construct a likelihood function for the probability that the observations are consistent with a given model configuration. The likelihood function enables the use of formal model calibration methods, such as Bayesian parameter estimation methods, to determine parameter values that are best supported by the observations, along with an estimate of the uncertainty in those parameters. This application of uncertainty quantification techniques to climate model development will be a unique and defining element of the atmospheric testbed. Pre-existing examples of climate model parameter optimization methods include a perturbed physics ensemble of the United Kingdom's Meteorological Office model (Murphy et al. 2004, Piani et al. 2005), an effort to tune CAM using climate integrations (Jackson et al. 2008), and other algorithms using data assimilation (Anderson et al. 2009) and model structure (Golaz et al. 2007). Our proposed data-driven model calibration will be unique in that our metrics are based on advanced process observations, as opposed to the general large-scale climate parameters used in a number of these prior efforts. We believe that it is more appropriate to calibrate parameters of a model's physics with observations of physical processes rather than with observations of large-scale climate. This hopefully reduces the chances of optimizing a model for the wrong reason. In essence, we aim to replace ad-hoc climate model tuning with a systematic and thorough parameter optimization process.

Before calibrating CAM with ACRF observations, we will perform an exploratory sensitivity analysis with a coarse 1° version of CAM5. This analysis provides: (1) the first-ever sensitivity analysis of CAM5, a model with many new highly-coupled physical parameterizations that may have different parametric sensitivities than earlier model versions; (2) a preliminary inventory of the physics parameters that may be responsive to the calibrations; and (3) a staging platform for specializing the numerical methods used in model calibrations. We will fully explore parameter space with nonintrusive sampling in order to build up stochastic expansion surrogate models such as polynomial chaos expansions. The surrogate models are computationally efficient statistical representations of the full climate model, and their expansion coefficients provide sensitivity and variance information (Tatang et al. 1997, Pan et al., 1997, Lucas and Prinn, 2005). Although CAM5 is a computationally intensive model, we estimate that existing LCF resources will be permit about 130 simulations of CAM5 in order to construct second-order stochastic expansions over fifteen uncertain parameters. If needed, anisotropic sampling techniques can extend the analysis to higher-order expansions or allow one to handle more uncertain parameters.

Once working in the calibration platform, two alternate techniques will be used to measure the robustness of the solutions to the UQ methodology. The first is to treat the parameter estimations as an optimization problem, where the goal is to find the values of physics parameters that minimize a set of defined objectives, such as the differences between model simulations and observations of Table IV.2. The second technique is the application of Bayesian inference methods, which require more careful customization and are more expensive but give accurate and detailed uncertainty information on the posterior distributions of the inferred parameters and in the (inferred) noise models for the data and model discrepancy. The posterior distribution of inferred parameters can be used to create sets of parameter values, rather than a single set, whose performance can be explored with limited integrations of the uniform high-resolution model in the validation platform. Both calibration approaches are computationally expensive if applied directly to CAM5; therefore, surrogate models for CAM will be built and used for parameter estimation. Because surrogate models can be evaluated very quickly, and because the choice of metrics affects the calibration process, we can explore the impact of using different techniques and combinations of metrics in the calibration platform.

The use of metrics in parameter calibration will likely incur large demands on both the metrics and numerical techniques used in parameter optimization. On the one hand, it will be necessary to quantify observational uncertainty in the metrics used. This is difficult since most climate observational data sets do not come with uncertainty estimates. However we expect that progress is possible as previously discussed (Section IV.2). On the other hand, metrics with diverse topology, such as the agreement with observations in the probability distribution function of precipitation rate and the mean diurnal cycle of precipitation, increase the complexity of the calibration problem. Another critical issue is the maximum number of metrics and perturbed parameters that can be optimized with a finite limit of computational resources.

In later years of the project, we envision using these uncertainty quantification techniques for more advanced questions. In particular, we will explore how the tuned values of parameters depend on model resolution or how they depend on the exact mathematical method of surrogate model fitting and ensemble generation. We will also test how calibration is sensitive to structural changes resulting from the use of alternate parameterizations. Another question worthy of exploration is the identification of which observations provide the most value in parameter optimization and what additional process-level observations would be most valuable to collect.

IV.4.1 Parameterization Development

While parameter optimization may be of great value once a model configuration has been determined, it cannot replace scientific insight in the model development process. Furthermore, parameter optimization may highlight physical parameters or whole parameterizations that are particularly flawed, but cannot provide the insight needed to develop improved model configurations. We thus expect parameterization development to be a vital part of this effort as we are pushing the parameterizations developed for low-resolution hydrostatic dynamics to their limit.

Despite this, we aim to adapt the existing parameterization suite of CAM5 in as straightforward way as possible–particularly for a climate model with resolution of 1/8°. We believe this is possible as the European Center for Medium-range Weather Forecasts performs its deterministic forecast with a model at T1279 (16 km) resolution using by-and-large the same parameterization suite used for many generations of the model at lower resolutions. Specifically, we will attempt to make small changes to the existing parameterization suite work well for the high resolutions we will employ. The minimum change we envision is the removal (or sharp curtailing at a minimum) of the deep convection parameterization, but maintenance of CAM5's shallow and boundary layer turbulence schemes as they parameterize the effects of motions on scales which are much smaller than the grid resolution of 1/8°. Additional changes that may be needed include the simplification of the cloud fraction parameterization in the stratiform cloud scheme and the conversion of stratiform precipitation from diagnostic to prognostic model variables. It is not envisioned that any significant changes are necessary to the existing aerosol physics and/or radiation schemes for the hydrostatic model. However, some aspects of the aerosol-cloud coupling such as the use of vertical velocity in nucleation parameterizations and washout of aerosols by precipitation may need examination. Nonetheless, we do not envision a major effort to develop new parameterizations from scratch.

Additional efforts may be needed in two other areas. First, we will explore increasing CAM's vertical resolution from 30 to about 50 to 80 levels. Second, the computational efficiency of existing CAM5 parameterizations may need improvement even if the deep convection parameterization is removed. We may need to develop accelerations for some physics routines and reformulate the physics to work on the same model state, rather than the current process-splitting, in order to permit greater concurrency.

IV.4.2 Uncertainty Quantification in Atmospheric Testbed Milestones and Deliverables

Year 1

- Initial surrogate model for prototype calibration platform
- Exploratory sensitivity analysis of low-resolution CAM5
- Determine CAM5 physics parameters to be perturbed and their ranges
- Address parameterization issues related to variable resolution grid and increased horizontal and vertical resolution, as needed

Years 2–3

- Define sets of parameter values with equal calibration platform metrics
- Explore the sensitivity of parameter sets to the method of surrogate model fitting
- Provide parameterization modifications to convection, cloud, and aerosol parameterizations as needed

Years 4–5

- Explore sensitivity of parameter sets to parent model configuration and the choice of site of interest
- Analyze of the relative value of calibration platform diagnostics to improvement in global climate simulation
- Limited sensitivity analysis of the high-resolution model utilizing parameter sets devised from calibration platform

Address parameterization computational efficiency issues as needed

V. CSSEF OCEAN AND ICE DEVELOPMENT

V.1 SCIENCE GOALS

Small spatial scales and very long time scales characterize ocean circulation. Ocean mesoscale eddies, with sizes of ~50 to 100 km, play a strong role in the global circulation of the ocean. Eddies can also directly affect atmospheric winds (Chelton et al. 2004) and the supply of nutrients for ocean ecosystems (McGillicuddy et al. 2007). Other important ocean processes, like deep water formation, occur at even smaller spatial scales. Resolving eddies has been shown to be a necessary condition for an accurate simulation of ocean circulation (Shaffrey et al. 2009, Hecht and Smith 2008, Hallberg and Gnanadesikan 2006, Maltrud and McClean 2005). The position and representation of Western boundary currents like the Gulf Stream are greatly improved in eddy-resolving models (Maltrud and McClean 2005), a result that could have a strong impact on the troposphere (Minobe et al. 2008). While fully coupled climate simulations with eddy-resolving ocean models have been performed (McClean et al. 2010), they remain too computationally expensive to perform for routine climate change experiments or ensemble simulation. Variable-resolution models, in which resolution can be focused in eddy-active regions, represent a promising approach for performing eddy-resolving simulations at much-reduced computational cost. Variable resolution can also be useful in the future to capture even smaller spatial scales or to perform regional studies in a global context.

While spatial scales are short, time scales can be long in ocean circulation. The thermohaline circulation (THC) transports water over time scales of many centuries to a millennium. Exploring the stability and long-term variability of the THC would require very long integrations. However, as resolution increases, the time step in explicit forward time integration must decrease. In a variable-resolution model, there are multiple time steps, and the finest resolution region will limit the integration. We will require alternatives to current explicit schemes to be able to integrate ocean (or ice) models for long periods to explore THC stability and centennial-scale climate change.

Like the ocean, sea ice dynamics are strongly influenced by small-scale processes. Sea ice is composed of a series of rigid floes from meters to 5 km in size. When a force is applied to these floes, either from a wind or ocean current, they are made to move. Two floes may diverge, generating open water between then (termed a “lead”). When leads are formed, the relatively dark surface of the ocean is exposed to local atmospheric conditions, causing either warming of the ocean or rapid freezing, depending on those conditions. Two floes may converge, in which case the ice will break up and form a ridge, or the floes may slide past one another. The rheology of the ice (Feltham 2008) is a description of how the ice responds to these stresses. Traditionally, sea ice has been treated as an isotropic continuum because the length scales of interest were large enough that a representative sample of floes and lead/ridge orientations were contained in a single grid cell. This will no longer be true as climate scientists increase resolution and new formulations of ice rheology are required to better represent ice dynamics. Better representations of the ocean-ice interface and stresses are also needed.

Under the CSSEF project, we propose to

- Accelerate development of a new variable-resolution ocean model by improving computational performance and developing new scale-aware parameterizations,
- Explore and implement new sea ice rheology formulations that are more appropriate for high-resolution simulations and develop improved methods for ocean-ice coupling,
- Introduce new Jacobian-Free Newton-Krylov solvers to provide more flexible and accurate time-integration schemes,
- Create a new ocean and ice model testbed for evaluating new model improvements, and

- Apply new uncertainty quantification (UQ) methodologies to inform parameter and resolution choices for ocean and ice models.

V.2. OCEAN MODEL DEVELOPMENT

As described above, improved ocean simulations follow from resolution of small-scale features, especially mesoscale eddies and topographic features. Eddy-resolving simulations within a coupled model are currently too expensive to integrate for ensembles of climate change scenarios. Variable resolution may provide a means to achieve eddy-resolving simulations at greatly reduced cost by focusing resolution on eddy-active regions and other regions where resolution has a strong impact (e.g., eastern boundary upwelling regions). As future computers permit high-resolution throughout the globe, there will continue to be unresolved features and processes that would benefit from a variable-resolution approach.

We are developing a next-generation climate-modeling framework based on variable-resolution, unstructured meshes using the Model for Prediction Across Scales (MPAS) framework. At the core of MPAS is a unique approach that combines a robust, variable-resolution meshing strategy for the sphere with state-of-the-art numerical methods applicable to such variable-resolution meshes within a global modeling framework.

The idea of decomposing (or tessellating) a region of space based on a Voronoi gridding strategy has been explored for more than a hundred years (Dirichlet 1850, Snow 1855, Voronoi 1907). Imposing a centroidal constraint (Du 1999, Du 2003, Ringler 2008) endows the resulting mesh with quality metrics that are superb and are arguably unmatched by other approaches to meshing the surface of the sphere. A user-defined density function allows the placement of resolution where it is required. For example, Figure V.1 depicts a global meshing of the sphere with one region of mesh refinement. Multiple regions of mesh refinement, each with arbitrary levels of refinement and arbitrarily smooth or rough transitions zones, are supported. The meshes are easily generated on typical desktops based on freely available software (Ringler 2008).

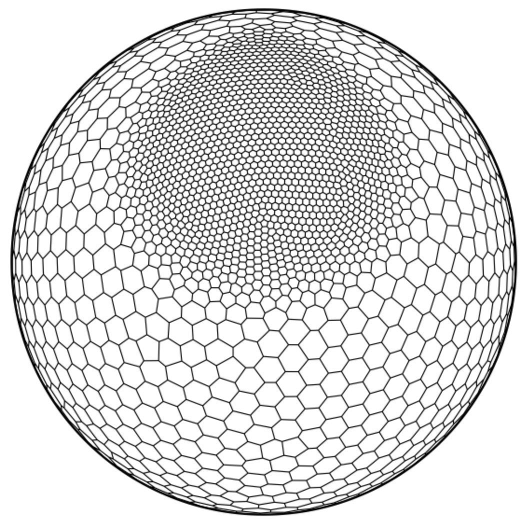

Figure V.1. A variable resolution grid based on a Spherical Centroidal Voronoi Tesselation.

The key breakthrough that enables the use of variable-resolution meshes for atmosphere, ocean, and ice systems is a robust multi-scale finite-volume technique (Thuburn et al. 2009, Ringler et al. 2009). The new finite-volume method generalizes the seminal work of Arakawa and Lamb (1981) to support a wide range of convex polygons (e.g., triangles, quadrilaterals, or Voronoi meshes) on multi-resolution meshes. The numerical scheme conserves mass and potential vorticity to within round-off error, conserves total energy to within time truncation error and dissipates potential enstrophy at a user-defined, mesh-invariant time scale (Sadourny and Basvedant 1985). The resulting approach allows for the simulation of realistic atmosphere and ocean flows on variable-resolution meshes without the need for ad hoc stabilization techniques in the mesh transition zone or elsewhere. We expect that this multi-scale finite-volume approach will excel at both quasi-uniform, high-resolution modeling as well as the exploration of regional climate processes within a global modeling framework.

The improvements described above are coded as part of a general MPAS software framework that can be used for any component model. The framework handles the vast majority of the software infrastructure needs: system builds, memory allocation and management, grid information, array declaration, data decomposition, message-passing interface (MPI) communication, netCDF (network common data format)-based restarts, and netCDF-based output. As a result, the MPAS global ocean model is currently constructed with just a few (currently four) additional source files. The entire framework holds for any mesh supported by the finite-volume technique.

V.2.1 MPAS Ocean (MPAS-O)

We have been developing an ocean model (MPAS-O) built on the MPAS framework. The variable-resolution approach will enable us to resolve features in the ocean at a greatly reduced computational cost, and the new ocean model takes full advantage of the improved numerical schemes described above. We have performed some initial tests using a full 3D (three-dimensional) global ocean configuration with simplified physics and idealized forcing. We are also actively working on new hybrid vertical grids based on earlier work for a prototype Hybrid Coordinate Parallel Ocean Program (HYPOP) model based on the Parallel Ocean Program (POP) framework.

Under the CSSEF project, we propose additional work necessary to transition this model from the prototype stage to a full production ocean model that performs well in a coupled climate model context. We will focus on two immediate challenges. First, current model development has directed toward an accurate working prototype with little consideration or attempt at optimizing computational performance. We will need to substantially improve the computational performance and throughput to be competitive with current models. Second, all of the testing to date has been with very simple physical parameterizations of mixing. We will need to adapt parameterizations to the new framework and additionally develop new formulations that can be used in a variable-resolution model that will resolve processes in some regions while needing to parameterize in others.

V.2.2 Computational Efficiency

The MPAS framework is designed to exploit the current generation of leadership-class high performance computing systems, utilizing domain decomposition and a flat MPI programming model. Standard tools like Parallel Graph Partitioning and Sparse Matrix Ordering (ParMETIS) (Schloegel et al. 2002) are used to generate optimal grid decompositions. However, MPAS performance lags well behind the current POP ocean model in a similar configuration. This is not surprising given the focus on a working prototype rather than on computational performance. Performance penalties can arise from a number of features in the current MPAS-O implementation. First, unstructured meshes like those in MPAS carry performance penalties because the indirect addressing required to encode references to neighboring cells is more inefficient that the predictable strides and indexing found in structured grids. These penalties are often offset by the other advantages of unstructured grids. In the ocean case, this includes complete elimination of land cells throughout the grid, where structured grid approaches often compute over land and mask the results. We will need to evaluate both positive and negative aspects of unstructured grids from a performance standpoint.

A second potential performance penalty may arise from data structures and index ordering. In the current POP model, horizontal indices are innermost as a result of choices in code structure, memory footprint and optimization of stencil operators. In MPAS-O, the horizontal index is outermost to provide optimization opportunities on new hybrid or graphics processing unit (GPU) accelerators, based on discussions with LANL Roadrunner experts. This new data structure and index ordering has not been fully evaluated to determine whether it presents a performance problem.

Third, the MPAS framework provides a very flexible and automated system for model configuration, memory allocation and runtime determination of a number of model arrays and parameters. While very nice from a user interface perspective, these choices may have significant performance penalties as a result of their implementation in user-defined types, data structures, and pointers. We will need to fully evaluate the performance implications of these flexible structures.

Finally, we will need to evaluate software needs for future architectures and anticipate those needs in our current design. All of the above will require a significant effort at profiling, optimizing, and refactoring code to achieve comparable performance to our current POP model that has been optimized over the past 15 years. This performance optimization will include both single-node performance as well as scaling and parallel performance on large core counts.

V.2.3 Scale-Aware Closures

In typical Intergovernmental Panel on Climate Change (IPCC)-type simulations, ocean eddy activity is entirely parameterized through the use of the Gent-McWilliams (GM) (GM 1986) closure. The GM closure, through the relaxation and flattening of the large-scale isopycnal surfaces, attempts to mimic the conversion of ocean available potential energy to ocean eddy kinetic energy. This energy conversion is accompanied by a poleward heat transport that is essential for the realistic simulation of the climate system. Since ocean eddy activity controls and/or mediates many of the dominant physical processes of the global ocean system, an accurate parameterization of eddies is essential for realistic simulations of the ocean system when eddies cannot be explicitly resolved.

In eddy-resolving simulations, parameterizations like GM are not required. One of the main motivations for MPAS-O is to provide the ability to directly simulate ocean eddy activity in large portions of the ocean domain. This capability will likely be of significant scientific value, but brings with it new challenges. Specifically, if eddies are directly simulated in one part of the domain and are parameterized in another part of the domain, we are obligated to develop parameterizations that “turn themselves off” as eddies transition from parameterized to resolved. This is essentially the challenge of developing scale-aware parameterizations. While this challenge is most pressing for eddy parameterizations like the GM closure, the challenge, in fact, extends to all ocean parameterizations with tunable parameters that vary as the mesh resolution changes. These include overflow parameterization, representation of topography, vertical mixing, tidal mixing, and submesoscale eddy parameterizations.

During the first half of this proposed effort, we will focus on the kinematic aspects of ocean closures, namely dispersive and dissipative closures that operate at or near the grid scale to control the accumulation of grid-scale energy. Particular focus will be the development of accurate closures in the presence of variable-resolution meshes. An initial implementation will rely on a new kinematic closure developed by Ringler and Gent (2010) that conserves potential vorticity based on either the GM approach or the Lagrangian-Averaged Navier Stokes (LANS) approach (Holm 1999, Hecht et al. 2008ab, Petersen et al. 2008). This new formulation is directly applicable, without alteration, to the variable meshes utilized by MPAS-O. An initial effort will be focused on a full scoping, testing and implementation of this new parallel vorticity (PV) closure in MPAS-O.

Following the evaluation of the new closure above, the scope of the scale-aware parameterization effort will broaden significantly to include overflows (Legg et al. 2009), sub-mesoscale eddies (Fox-Kemper et al. 2008) and tidal mixing parameterizations (Jayne and Laurent 2001). Each of these parameterizations will have to be evaluated for their respective sensitivity to grid resolution. The ultimate goal, that will require sustained development beyond this 5 year effort, is the creation of a full suite of ocean model parameterizations that can be formulated in a robust, scale-insensitive manner.

V.3 SEA ICE MODEL DEVELOPMENT

For future generations of the Community Earth System Model (CESM), there are two focus areas for sea ice model development. The first involves the appropriate coupling for oceans and ice, especially the dynamical coupling at the ocean-ice interface that impacts the momentum transfer and pressures at that interface. The second addresses the need for a new dynamical formulation for high-resolution sea ice models.

V.3.1 Ocean-Ice Coupling

Ocean and sea ice models in the CESM are currently treated as separate components, primarily as a result of the historical development of the two as stand-alone components. The ice is assumed to float on the surface of the ocean with a uniform interface between them. The ocean model is responsible for all liquid water and passes a total frazil ice volume to the sea ice model, computing that volume based on the amount of freezing necessary to keep the ocean temperature at the freezing point. The sea ice model handles all ice freezing and melting, providing the resulting heat and water flux back to the ocean model. While the present coupling interface has been adequate for many climate simulations, there are several weaknesses with this approach that will need to be addressed in future models. We propose here new approaches to ocean-ice coupling to address these weaknesses.

The first weakness in the approach is related to the freshwater exchange at the ocean-ice interface. The current POP ocean model is a constant-volume formulation and treated freshwater flux as a virtual salinity flux, converting the volume of freshwater into an equivalent salt flux. This formulation captured the salinity changes in the ocean while preserving the constant volume assumption. A variable-thickness surface layer was added to POP several years ago to enable a true freshwater flux as long as the flux was not large enough to deflate that surface layer or that the surface height change was small compared to the thickness (a linearization condition for the implicit free surface formulation). While this new addition allowed for a more realistic freshwater flux due to ice freezing/melting, the change in surface height generates a pressure gradient that drives ocean currents. In the real ocean, these pressure differences are compensated by the change in the weight of the sea ice at the surface of the ocean. There should be no change in total pressure in the combined ocean-ice system. The current ocean-ice coupling cannot account correctly for the changes in sea ice thickness to compensate for the changes in sea surface height as a result of freshwater fluxes due to melting and freezing of sea ice. The new MPAS ocean model conserves mass rather than volume, so better represents a true freshwater flux boundary but still does not account for the weight of the ice when coupled to an ice model.

A second factor in the dynamical coupling of ocean and ice is related to the momentum transfer at the ocean-ice interface. Because sea ice floats in the ocean rather than on the surface, seawater laps at the sides of ice floes, and the ice can carry some of the surface ocean mass as it moves. This is especially true when ice is melting, and there is a boundary layer of relatively fresh water under the ice that partially decouples the surface ocean-ice layer dynamics from the underlying ocean. The mass of the ice cannot simply be included in the surface ocean as a liquid with the standard atmospheric forcing at the surface because the material properties of the ice respond very differently to the surface wind stress. The transmittance of surface wind stress to the deeper ocean is greatly influenced by the combined ocean-ice boundary layer that includes seawater within leads, the ice matrix itself, and the thin boundary layer of modified-density seawater just beneath the ice. This interface is particularly important in the Arctic, where the ice motion has a strong inertial component. Wind stress is currently applied at the surface of the ice and the surface of the ocean, and the stresses are averaged based on ice fractions. The ocean-ice stress is computed using a simple quadratic drag that is highly idealized. Because the ice thickness is not regular and the ice penetrates into the surface ocean, the ocean currents can force the sea ice from horizontal transfer of momentum at the sides. As mentioned above, the ice can similarly force surface ocean water and can drag this water with it as it moves in response to wind stress. None of these effects are adequately treated in the current assumption of a smooth layer of ice floating on the ocean surface.

In addition to the momentum transfer, there are thermodynamic implications of a more complicated ocean-ice interface. A significant issue is the assumption that the interface between ocean and ice is a solid-liquid boundary governed by a phase change due to melting and freezing of water. Sea ice is not just solid ice – it includes brine. When the ice is very cold, brine in the ice interior is isolated from the ocean, but often the brine could be considered an extension of ocean water into the ice. In the water-ice slurry that is present as ice freezes, seawater flows upward into the mixture (a mushy layer), and becomes more dense as it cools and concentrates, as ice crystallizes from it. This heavier brine then partially drains out of the freezing layer, completing a convective cycle. During warmer times of year, sea ice becomes permeable, allowing fresh surface melt water to flush through interconnected brine channels into the ocean, or for oceanwater to be forced upward through the ice to the surface under a heavy snow load or around ridges. These processes are critical for biogeochemical cycling within the sea ice and for ice-related chemical and biological changes in the ocean. They also create difficulties in defining the ocean-ice interface because the solid ice fraction declines smoothly to zero with depth in the ocean.

While there are current parameterizations being developed for sea ice hydrology and brine issues as well as the momentum coupling, it is clear that the ocean-ice interface is not a clean interface and not well represented by current coupling assumptions. Both sets of problems point to the need for a more tightly coupled description and formulation of the ocean-ice boundary layer. We propose to explore embedding the sea ice code within the ocean model. This approach would enable a more accurate treatment of a variety of interface issues. An additional benefit would be that an embedded ice model would immediately gain the advantages of the MPAS ocean in terms of variable resolution and other numerical improvements. The spatial (and time) scales of these boundary processes are much smaller than those generally modeled in the surface ocean, however, and it seems unlikely that the ocean and ice equations themselves would be combined. Ice processes are likely to continue as separate parameterizations but with a more cohesive and clever coupling strategy with the ocean model. That strategy is yet to be determined and would be the focus of this effort. Potential approaches could leverage current efforts (under the Investigation of the Magnitudes and Probabilities of Abrupt Climate Transitions [IMPACTS] project) to simulate the ocean-ice sheet boundary under grounded ice sheets using embedded boundary layer models. A unified approach to both of these ocean-ice interfaces will be a goal of this effort and will include additional ocean-ice shelf work in future years. For the time coupling, we will explore novel techniques described in the time integration section below.

V.3.2 Anisotropic Rheology of Sea Ice

The Los Alamos sea ice model, CICE, currently uses an isotropic continuum rheology. More specifically, the ice is treated as a plastic material that undergoes failure at some critical stress. Beyond this stress, the ice creeps viscously under an applied load. Some elastic behavior is also allowed for numerical reasons (Hunke and Dukowicz 1997).

As the horizontal resolution of simulations increases, continuum isotropic models are becoming less representative of sea ice. For grid cell sizes smaller than 10 km, too few leads are present in each cell for the ice to be treated as isotropic. Linear kinematic features are a ubiquitous feature of Arctic sea ice that requires an anisotropic rheology to explain properly. These are long and narrow regions of strong ice deformation several hundred kilometers in length that are likely to be regions of strongly aligned leads and ridges.

Several attempts have been made to develop anisotropic rheologies for sea ice, but these are often too expensive numerically for inclusion in a global climate mode. An example of this would be the granular model of Hopkins (Hopkins 2004). Other anisotropic models may be suitable for inclusion in a global climate model. Schreyer et al. (2006) developed an elastic-decohesion model of sea ice failure. Here, the point at which the ice fails and a lead is formed is determined along with the lead orientation, width, and mode of failure. Wilchinsky and Feltham (2004) describe the rheology in a different way. In their model, the grid cell is divided up into many subelements, each of which contains a single lead with some orientation. The orientation of the leads can change within each subelement as they respond to the applied stress. Averaging the behavior across all the subelements determines the rheology.

We plan to include an anisotropic rheology into CICE, first to determine whether anisotropic features of sea ice, such as linear kinematic features, can be accurately simulated with these new rheologies, and then to evaluate the effect this has in high-resolution simulations.

V.4 OCEAN AND ICE TIME INTEGRATION

As noted above, the long time scales associated with the ocean thermohaline circulation, time step restrictions in high- or variable-resolution models, and the future need for nonhydrostatic formulations all require a new approach to time integration in ocean and ice models. We require a flexible time integration scheme that enables some choice in how to represent multiple time scales. Having the ability to perform climate simulations with reduced splitting errors and using variable-resolution grids will be a significant step forward in predictive ocean and sea ice simulation.

We propose to implement a fully implicit, Jacobian-Free Newton-Krylov (JFNK) (Knoll 2004) option within both the new ocean model (MPAS-O) and sea ice (CICE) model. The JFNK framework allows tighter coupling of the physics, thus reducing errors and increasing stability inherent to operator splitting. In addition, higher-order implicit time integration schemes are easily implemented in the JFNK framework. When globalized, JFNK exhibits enhanced robustness with improved convergence properties. The need for globalization was clearly established in Lemieux (2010).

The key to efficient implementation of JFNK is effective preconditioning. In the proposed work, “physics-based” preconditioning (Knoll 2004, 2005) will be employed. This unique preconditioning approach is a highly successful and proven approach for effective preconditioning for multiple time scale problems where an accurate simulation is desired on the dynamical time scale. Simultaneous gains in efficiency and accuracy have been documented in a wide variety of stiff wave fluid dynamics problems, including 3D parallel examples in hurricane simulation (Reisner 2005) and magnetohydrodynamics (Chacon 2008). Furthermore, these gains have been understood through a modified equation analysis of splitting and linearization errors (Knoll 2003).

Following the standard prescription for physics-based preconditioning, we will reformulate the current ocean simulation semi-implicit solver (Dukowicz 1994) as a preconditioner, and we will reformulate the elastic-viscous-plastic (EVP) sea ice solver (Hunke and Dukowicz 1997) as a preconditioner. When done appropriately, the physics-based preconditioner can then be used as either a preconditioner or a solver. This leaves both semi-implicit and fully-implicit options available to the user. JFNK implicit solvers have been developed for both ocean circulation (Weijer 2009) and sea ice modeling (Lemieux 2010). In both cases, more traditional preconditioners have been applied. Our development of more advanced, physics-based preconditioners will leverage the SNL scalable solver package, Trilinos (Heroux 2003), used for optimal scaling technology, and similar concurrent work to be done in the atmospheric Community Climate System Model (CCSM) component at ORNL. We already have a highly qualified team in place with expertise in these techniques at LANL, ORNL, and SNL.

We reemphasize that the combination of JFNK and physics-based preconditioning is a highly proven, well-tested, concept, and thus a fairly low-risk, high-return endeavor. In a well-documented study, a compressible, 3D, multiphase, numerical model of a hurricane demonstrated significant efficiency gains for equal accuracy using physics-based preconditioning and JFNK (Reisner 2005) as compared to the more standard semi-implicit-based solver. Splitting and linearization errors in the semi-implicit method render it less accurate as the time step is increased above the stiff wave time scale. This is the case even though the semi-implicit method remains numerically stable. It has been shown via numerical analysis that these time integration errors are not present in the fully implicit approach (Knoll 2003), thus allowing for larger time steps with increased accuracy.

Additional arguments can be made for fully implicit JFNK-based methods in ocean models for long time integration applications such as spin-up and for improved time coupling to other models such as sea ice. Thus, this effort to include a fully implicit JFNK-based capability will provide an indispensable tool for model development at higher resolution. With a JFNK solver, the desired solution is time-step converged when taking time steps on the order of the dynamical time scale, a crucial feature as we scale to exascale simulation.

Finally, once methods are implemented in both ocean and sea ice components, we will investigate the use of nonlinear elimination (Lanzdron 1996) to improve the coupling between the ocean and sea ice components. Nonlinear elimination requires the formation or approximation of a matrix-vector multiply of the coupled system, and thus fits naturally in the JFNK framework. This option for coupling becomes available to us when we have a JFNK-based solver for ocean and sea ice components.

V.5 OCEAN AND ICE TESTBED DEVELOPMENT

In order to validate our new ocean and ice models, we will need to develop a complete model validation suite. Ocean and ice models lack the comprehensive metrics and frameworks for evaluation and validation that exist for the atmosphere model. Currently, ocean and ice models are validated against observational data for global simulations of current climate. While this is important, such a validation cannot account for compensating errors and cannot verify the accuracy of particular process representations. We require a comprehensive ocean and ice testbed environment through which routine evaluation of ocean and ice processes can be undertaken.

The testbed will include a hierarchy of tests. At the lowest level, simple unit tests will verify the correctness of software infrastructure, numerical operators, and equations of state. A second level of testing will evaluate advection, transport, and process parameterizations. For these tests, ocean and ice model evaluation problems have been published in the literature or on line. We will gather these test cases and develop new test cases, as necessary. In addition, we will compile or generate the appropriate reference solutions (analytically or with reference model calculations). Example test cases include dynamical tests (e.g., shallow water and advection tests), error growth, interactions with bottom topography (e.g., overflow and sea-mount tests), vertical and horizontal mixing parameterizations and simple basin configurations (e.g., double-gyre). Finally, testing of the full model in global or regional configurations will be needed. Standard configurations like those defined by the Arctic Ocean Model Intercomparison Project (AOMIP) or the Common Ocean Reference Experiment (CORE) can be used.

Tests of the full models will be evaluated against observational data sets. The Climate Variability and Predictability (CLIVAR) Working Group on Ocean Model Development publishes a Repository for Evaluating Ocean Simulations (REOS) (CLIVAR 2010), a compilation of links to various scattered data sets useful for ocean-model evaluation. The complete list of data is available at http://www.clivar.org/organization/wgomd/reos/data sets.php. In addition, AOMIP (http://fish.cims.nyu.edu/project_aomip/overview.html) has defined standard test problems for model intercomparison in the Arctic. We will need to aggregate data sets from these sites and generate appropriate metadata for use in our testbed framework. Also, some of the data sets come from floats, buoys and other non-gridded and even non-stationary data. In some cases, research teams are already creating gridded data sets based on those, but in other cases, we will need to interpolate that data to grids for model-data intercomparison.

We will combine the tests described above into an automated validation testbed. The low-level verification unit tests will be combined into a standard regression test for use in the code development pipeline. For process testing and full model tests, we propose to create a validation testbed by combining the necessary scripts, model forcing and validation data sets as part of the overall CSSEF testbed and data repository development. We will collaborate with the testbed developers to aggregate and publish the appropriate data sets as well as develop standard scripts and interfaces for our test suite. At the end of the proposal period, we will have in place an initial automated test suite for ocean and ice model verification and validation upon which we can continue to add new tests and data as needed.

V.6 OCEAN AND ICE UNCERTAINTY QUANTIFICATION

To provide confidence in climate model projections, we would like to be able to measure the uncertainty in our simulation results. This is especially difficult for the ocean model as relatively few metrics can capture ocean circulation, and it is difficult to define appropriate measures for uncertainty. For example, a persistent bias in ocean circulation is the behavior of the simulated Gulf Stream and North Atlantic current system. In coarse-resolution models, the Gulf Stream does not separate from the continent at Cape Hatteras as observed and does not turn northwest around the Grand Banks. Instead, the current extends further northward and then proceeds too zonally across the North Atlantic. These pattern changes are difficult to quantify. A first task for uncertainty quantification is then to define appropriate metrics to measure how well the model represents the real ocean, especially invariant metrics for features, feature location, transport diagnostics, and eddy-relevant metrics like eddy spectra and kinetic energy. Because this is also a component of the testbed development described above, significant interactions between the two efforts will be required.

Once appropriate metrics have been defined, we will begin to use new uncertainty quantification tools to inform the model developments described above, namely scale-aware parameterizations, variable resolution, sea ice coupling, and ice dynamics. An early target will be the assessment of model sensitivity to eddy parameterizations and the optimal choice of parameters that yield the best solution. Under a previous project, we configured our current POP model in a channel test and began to apply UQ tools to assess the parameter sensitivity of the LANS-alpha closure. Metrics being examined are potential temperature vs depth, kinetic energy and eddy kinetic energy, and the depth and spatial trend of isotherms. This simple case provides a useful configuration for testing the methodology and exploring the appropriate parameters in an unresolved configuration compared to a fully resolved nonparameterized solution and enables the generation of a large ensemble. To explore a variable-resolution implementation, we will extend this work by first adding partially resolved solutions to the current set of experiments. Once new parameterizations have been implemented in the MPAS-O model, we will repeat these experiments and add a new variable-resolution configuration to inform how parameters should scale as a function of resolution. Finally, we will extend this work into full global configurations of the MPAS-O model and explore multiple eddy parameterizations. This staged approach will permit the evaluation of UQ methodologies while also accommodating the model development timeline for the MPAS-O model.

Another application of UQ will be the exploration of model sensitivity to choices of variable resolution meshes. We will need to examine the response of the model as we focus resolution in particular regions. The hypothesis driving a variable-resolution formulation is that we can achieve a better simulation without utilizing high resolution throughout the domain. This assumption will need to be quantitatively evaluated by exploring different meshes that focus resolution in regions that are expected to be important. Some examples include a focus on Western boundary currents, Eastern boundary upwelling regions, the Southern Ocean and equatorial current systems. In addition, a mesh that is based on sea surface height variability (as a proxy for eddy activity) will be tested. The response of these simulations compared to a uniform high-resolution solution will help to quantify the uncertainty related to resolution in a variable resolution model and inform the cost/benefit tradeoff in adding grid resolution.

Related to grid resolution is the representation of bottom topography. Topographic features can significantly impact simulation results and improved representation of bottom topography in a high-resolution model is known to contribute to improved results at higher resolution. However, this improvement has not been quantified. Because a fine resolution grid can be configured with coarse resolution (or smoothed) bottom topography, the relative contribution of improved bottom topography to a high-resolution simulation can be isolated and quantified. A set of high-resolution simulations with different representations of bottom topography could be used to quantify this aspect of model improvement.

Applications of UQ methods to sea ice model development will also be explored. Ice extent (minimum and maximum extent), ice thickness and ice transport provide useful metrics for evaluating sea ice model performance. New formulations for ocean-ice momentum transfer and other ocean-ice boundary processes will likely provide more opportunity for parameter sensitivity. Similarly, anisotropic rheologies will need to be calibrated as they have not been extensively tested or used in global models to date.

The root of model UQ is comparison with the real system. Only in comparison with observations can we assess simulations, resulting in models of their accuracy and bias, calibrated input settings, and overall likelihood for estimating states of the system. A large part of the Ocean UQ challenge is establishing observation data sets and metrics (as related in the testbed goals) that are most relevant to the desired estimates and projections. In the ocean problem, we can also in some cases leverage very high-resolution simulation results to use as targets for lower-resolution simulation grids, as they are able to match the real ocean with greater fidelity in some measures.

UQ methods to accomplish these goals will rest on the established techniques of surrogate modeling of complex simulations. This approach uses an ensemble of runs covering a state space of interest (either simulation inputs or parameterized boundary conditions). This ensemble is used to characterize the response of the simulation, and is approximated by a simple, fast surrogate response function, such as a Gaussian process. This surrogate can then be used for Monte-Carlo analyses that cannot be carried out against the full, computationally expensive simulation. The analyses that can be performed include sensitivity analysis, understanding how inputs and combinations of inputs impact model response; inverse analysis or calibration, finding what settings of inputs are compatible with target responses such as observations; analysis of expected model discrepancy; state-space integrations (e.g., quantile estimation); and projections of the response distribution consistent with the uncertainty established in all of these sources. The final step usually involves running a small sample of simulations to validate the projections estimated with the surrogate.

V.6.1 Experimental Plan

Most of the model development activities and validation can be performed with short simulations and on resources currently available as part of DOE Office of Biological and Environmental Research (BER)-funded resources for this purpose. High-resolution reference solutions also exist from a previous 120-year eddy-resolving simulation. However, for a clean comparison, at least one new high-resolution solution using the new MPAS model will need to be generated, requiring approximately 12M core-hours based on current POP 0.1-degree results on ORNL LCF resources.

Most of the significant simulations will arise in the context of UQ, where ensembles that explore parameter space are required. These simulations will not occur until Year 3 and later, since much of the early UQ ensembles will be in the context of simpler test configurations. After Year 3, we anticipate the following experiments, subject to change based on Year 1–2 results.

For ocean parameter estimation and sensitivity studies, we anticipate using coarse and variable resolution MPAS ocean in relatively short (20–30 year) simulations. It is likely that this will be ~50 member ensemble. Based on POP 1-degree global simulations at the ORNL LCF, we estimate this will require ~500,000 node-hours.

A similar effort will be required for sea ice model parameter estimation. In this case, high-resolution simulations in an AOMIP configuration can be used and for a few decades of simulated ice. Costs for the new ice model dynamics and boundary schemes will likely increase over the current model, so we estimate ensembles would cost ~10M node-hours.

Finally, an exploration of resolution and topographic sensitivity will require a smaller ensemble (15–20) of mixed high- and low-resolution simulations for a few decades each. These will require an additional 10–20M node-hours.

V.6.2 Ocean and Ice Milestones and Deliverables

Year 1

- Initial performance profile for prototype MPAS ocean model and identification of performance limiters
- Implement new kinematic closure for MPAS ocean model and begin design of multi-resolution approaches
- Formulate initial design of new ocean-ice interfaces and develop potential approaches for new momentum and tracer coupling at the interface
- Evaluate candidate rheologies and create plan for integrating and testing new approach in CICE
- Implement initial preconditioner in implicit version of POP model to test approaches. Begin design of implicit sea ice software design
- Identify the initial set of model test configurations and reference solutions for validation testbed and begin creation of unit and process level test drivers
- Identify model quality metrics for ocean and ice for the UQ applications
- Generate initial results from UQ application to POP LANS-alpha in a channel configuration and sea ice parameterization in a reduced resolution configuration

Years 2–3

- Fix initial performance issues with MPAS ocean model with a goal of performance equivalence to POP in similar configurations. Identify cost-benefit of advanced schemes (e.g., new transport algorithms are likely to be more costly, but deemed worthy of that cost)
- Implement additional closure schemes for MPAS-O and evaluate results at IPCC-resolutions
- Initial implementation of CICE within MPAS framework and begin testing of ocean-ice coupling ideas
- Initial implementation of new sea ice rheology
- Implementation of split-explicit and semi-implicit preconditioned time integration in experimental branch of MPAS
- Implement capability of using EVP as a preconditioner to JFNK and Trilinos solver capability in sea ice component
- Complete prototype hierarchy of ocean test cases for validation testbed and begin development of automation scripts
- Complete reference UQ analysis of POP-alpha and sea ice; POP projection uncertainty ensemble available for analysis
- Begin application of UQ methods to new MPAS closure schemes
- Design and begin ensemble experiments for evaluating resolution and topographic sensitivity in UQ framework

Years 4–5

- Continue to optimize MPAS-O model and MPAS framework with an additional focus on new hybrid architectures to be delivered in Year 5
- Develop new scale-aware parameterizations for remaining physical processes represented in MPAS-O (e.g., overflows, tidal mixing, sub-mesoscale processes)
- Evaluate embedded sea ice model in ocean and related boundary schemes in full ocean-ice coupled simulations
- Evaluate new anisotropic ice rheology in full sea ice model
- Develop and implement globalization methods for JFNK and development of JFNK technology focused on the advanced models and discretizations as applied to sea ice problems
- Complete a fully automated ocean-ice validation framework
- Demonstrate ability of UQ framework to provide parameter estimation for closure schemes
- Use UQ framework to identify regional resolution sensitivity in MPAS ocean

VI. LAND SURFACE PROCESSES AND MODELING FOR CSSEF

VI.1 SCIENCE GOALS

A central objective of our efforts with CSSEF is to arrive at a detailed quantification of Earth system model prediction uncertainty. Using a new efficient testbed framework to integrate multi-dimensional model optimization studies, we expect to not only quantify but also significantly reduce prediction uncertainty associated with land processes. These optimization studies will take advantage of new approaches for organizing complex observational data sets.

The emergence of clear anthropogenic effects on the present-day climate and the increasingly detailed model-based expectations of likely future effects are leading to new questions about the structure and functioning of terrestrial ecosystems and their relationships to land physical environment and climate. The interactions of most interest from a climate-modeling perspective are those that affect the evolution of the climate system, particularly the coupled dynamics of carbon, nutrient, and hydrologic cycles on land and their interactions with the atmosphere. Carbon-climate feedback dynamics were identified in the Intergovernmental Panel on Climate Change (IPCC) Fourth Assessment Report (AR4) (IPCC 2007) as a critical area of uncertainty affecting predictions of atmospheric CO_2 concentration over the coming century. AR4 identified important controls on carbon-climate feedbacks associated with the hydrologic cycle, and acknowledged a potential role for carbon-nutrient interactions, but the necessary research foundations were not in place at the time to quantify these effects. Post-AR4 development in the Community Land Model (CLM) has focused on improvements in soil/snow hydrology, and on the introduction and evaluation of coupled carbon-nutrient dynamics, with the goal of providing initial quantification of the carbon cycle feedback.

While the post-AR4 research agenda has begun to identify these issues as being of particular importance, their development in the current version of CLM, and incorporation into the overall CCSM/Earth System Model (ESM), is still rather crude, and we do not understand how the current version of CLM contributes to the overall performance of the fully coupled model, or to overall prediction uncertainty. We will focus our efforts on two research areas where we believe climate prediction uncertainty is driven by a lack of integration and synthesis of existing process-level knowledge into current land model components of Earth system modeling frameworks, as captured by the following research questions:

- What are the magnitudes and dynamics of land-climate feedbacks?
- How do land subgrid hydrologic processes affect land-atmosphere interactions?

For land-climate interactions and feedbacks, our major emphasis here is on understanding how different natural and anthropogenic processes change over time, and therefore, how they affect climate prediction uncertainty through the evolution of climate-biogeochemical relationships and the carbon cycle feedback. For subgrid hydrologic processes, the major emphasis is on a more sophisticated representation of those processes and associated uncertainties over short time scales, to ensure that there is a more realistic representation of the hydrologic cycle in the overall Earth system model.

VI.1.1 Current Status of CLM4

The CLM, version 4 (CLM4) (Oleson et al. 2010), is the land component of both the Community Climate System Model, version 4 (CCSM4), and the Community Earth System Model, version 1 (CESM1). CLM4 includes a fully prognostic treatment of surface energy, water, carbon, and nitrogen fluxes and state variables for both vegetated and nonvegetated land surfaces. Recent model development includes improved surface energy partitioning and thus water cycling (Lawrence et al. 2007, Stöckli et al. 2008), and improved ability to reproduce contemporary global patterns of burned areas and fire emissions (Kloster et al. 2010). Subsurface hydrology parameterizations have also been changed to improve prediction of permafrost dynamics (Lawrence et al. 2008).

The coupled carbon and nitrogen cycle biogeochemistry functionality of CLM4 is an optional component, designated CLM-Nitrogen Cycle (CLM-CN), and all land modeling effort described in this proposal is performed with CLM-CN active. CLM-CN estimates states and fluxes of carbon and nitrogen for vegetation, litter, and soil organic matter, and associated exchange with the atmosphere (Thornton et al. 2009, Thornton et al. 2007). When activated, CLM-CN replaces the diagnostic treatment of vegetation structure (e.g., leaf area index, canopy height) in CLM with prognostic variables. For global gridded applications, the distribution of subgrid fractional area assigned to individual plant functional types is provided as an external forcing. CLM-CN includes a new approach to canopy integration that relates the sub-daily prediction of photosynthesis in sunlit and shaded canopy fractions to prognostic quantities for total leaf carbon and nitrogen through the assumption of a canopy gradient in specific leaf area (Thornton and Zimmermann 2007). The major components of CLM-CN include (1) a carbon cycle module linking pools (soil, litter, plant) with the atmosphere and simulating their exchange fluxes (e.g., photosynthesis, litterfall, decomposition); (2) a nitrogen cycle module linked internally to the carbon cycle and also to external pools; (3) a dynamic natural vegetation model to simulate prognostic vegetation structure and succession; (4) a prognostic model component for wildfire.

VI.1.2 CLM Development Efforts Under Way

It is important to note the developments already under way that are likely to be included in future versions of CLM and that will form the foundation for our intensive development work. The following broad categories of major model development are sufficiently advanced that it seems reasonable to plan around them as components of the next release of CLM (CLM5).

- Efforts to introduce new high-latitude processes, focusing on permafrost dynamics, thermokarst formation, improved lake biophysics, and new subsurface physical and biogeochemical dynamics necessary for prediction of methane emissions.
- Efforts to introduce a prognostic land use and land cover change capability, by integrating relevant algorithms from the Global Change Analysis Model (GCAM) Integrated Assessment Model (Brenkert et al. 2003, Clarke et al. 2007, Kim et al. 2006) and land use harmonization approaches (Hurtt et al. 2006) within CESM/CLM. These prognostic approaches will substitute for prescribed land use/land cover change data sets operational in CLM4, and are intended to improve the consistency between climate system evolution and human land use decision-making under future scenarios. This effort also includes coupling of the GCAM energy technology and energy use components directly within CESM.
- Efforts to develop a robust single-point modeling capability, with added parameterization flexibility necessary to represent detailed site characteristics, such as soil texture, land use and disturbance history, and experimental manipulations such as enhanced CO_2, warming, nutrient additions, and soil moisture manipulations. These efforts are leading to early exploration of parameter optimization and data assimilation with CLM4.
- Expansion of the existing Carbon Land-Modeling Intercomparison Project (C-LAMP) model-data evaluation metrics (Randerson et al. 2009) to include new data sources from tropical carbon-nutrient interaction experiments, temperate forest disturbance history and biomass observations, and high-latitude data sets on snow extent and albedo, permafrost extent and active layer depth, soil organic matter content, methane emissions, and fire extent and severity.

Ongoing work in each of these areas will be explicitly leveraged by the efforts proposed here, adding value to previously funded work through integration and depth of effort.

VI.2 DETAILED APPROACH TO LAND SCIENCE QUESTIONS

In the following sections, we provide details of our approach to addressing the two basic research questions for land model prediction uncertainty:

- What are the magnitudes and dynamics of land-climate feedbacks?
- How do land subgrid hydrologic processes affect land-ocean-atmosphere interactions?

Each science question is broken down into multiple topics, with specific approaches and deliverables for each topic. Descriptions in this section focus on specific land process details, with explicit connections to common uncertainty quantification (UQ) methods and data requirements, each of which is covered in more detail in subsequent sections.

VI.2.1 Magnitudes and Dynamics of Land-Climate Feedbacks

Land ecosystems influence the Earth's climate system through multiple biophysical and biogeochemical feedback mechanisms. These mechanisms operate mainly through net land surface fluxes of greenhouse gases (GHG), variation in land surface albedo, and land-atmosphere exchanges of sensible and latent heat. A major objective in the development of CLM4 was to improve prediction of future states of the climate and ecosystems by including new components and processes that contribute to these feedbacks. For example, estimating the sign and magnitude of the land component of the global carbon-climate feedback depends on a mechanistic representation of carbon uptake by vegetation, turnover of live plant parts to litter, and decomposition of litter by soil heterotrophs, with return of carbon to the atmosphere by respiration and long-term storage of recalcitrant forms of organic matter in soils. These dynamics are sensitive to spatial and temporal patterns of changing temperature and precipitation, which in turn depend on changes in GHG concentration, resulting in a complex array of feedbacks.

Recent work has shown that carbon-nutrient interactions are also likely to influence the expression of these feedback mechanisms, with variation in space and time as a function of mean climate, climate change vectors, vegetation type, and soil physical characteristics (Sokolov et al. 2008, Thornton et al. 2009, Zaehel et al. 2010). CLM4 includes a detailed representation of these mechanisms, but there are several areas where the current model structure has known or suspected deficiencies. Based on previous analysis of partially and fully coupled simulations at the global scale (Thornton et al. 2007, Thornton et al. 2009), and on sensitivity analyses performed at the site scale (Thornton et al. 2002), we identify four areas for investigation of model prediction uncertainty that relate directly to land-climate feedbacks, and for which we expect to be able to make robust and quantifiable improvements over the next 5 years. These four areas are:

1. Mechanistic models of litter and soil organic matter dynamics,
2. Mechanistic treatment of multiple nutrient limitations and carbon-nutrient interactions,
3. Prognostic subgrid age-class distributions, and
4. Prognostic land cover and land use change.

Details for each topic are given in the following sections.

VI.2.2.1 Litter and Soil Organic Matter Dynamics

The current arrangement of litter and soil organic matter (SOM) pools in CLM is empirically derived from radio-labeled substrate decomposition experiments carried out under controlled conditions in microcosms (Thornton and Rosenbloom 2005). The resulting structure is a converging trophic cascade (Figure VI.1) that represents heterotrophic respiration at multiple stages, with long-term accumulation of SOM dictated mainly by the dynamics of secondary (and higher-order) decomposers (i.e.,

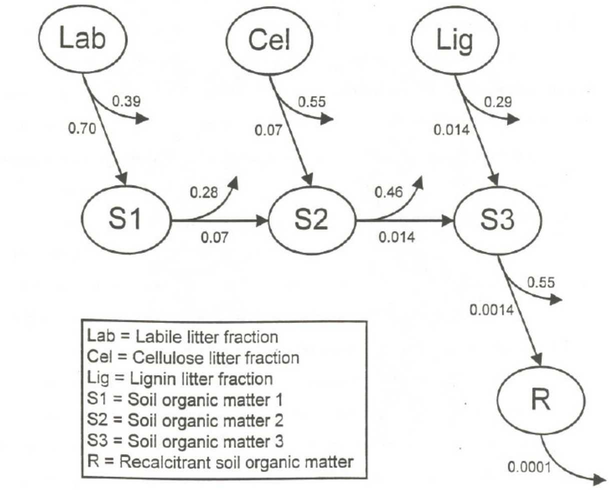

Figure VI.1. Trophic cascade model of litter and SOM pools in CLM4. Straight arrows indicate transfer between pools, mediated by microbial metabolism of organic matter from the upstream pool, resulting in new organic matter accumulation (metabolic byproduct) in the downstream pool. Curved arrows represent heterotrophic respiration losses of CO_2. Values on transfers are in units 1/day, values on respiration are carbon loss fractions.

microorganisms metabolizing organic matter from other microbial communities, as opposed to primary plant litter components).

While the structure and dynamics of this model are faithful to the radio-labeled substrate decomposition data used in its construction, richer data sets and more advanced methods are now available, suggesting some important structural and functional modifications which would impact prediction uncertainty. For example, results from the Enriched Background Isotope Study (EBIS) show that at the very least the model structure needs to include a representation of two sets of litter inputs, one aboveground for leaf (and woody) inputs, and another within the mineral soil layers associated with root inputs (Tipping et al. in review). New methods have improved our understanding of the chemical composition of stabilized SOM (Amelung et al. 2008, von Lutzow et al. 2006, Marschner et al. 2008, Kleber and Johnson 2010). Investigations of the chemical composition of mineral-associated organic carbon (MAOC) show that it is the mineral association itself and not the chemical composition which leads to long-term stabilization of certain fractions of the bulk soil organic matter (Kahle et al. 2004, Kleber et al. 2004, Kleber et al. 2005, Masiello et al. 2004, Mertz et al. 2005, Mikutta et al. 2006, Rasmussen et al. 2005, Torn et al. 1997). We also expect that changes in soil oxygen saturation state with depth in wet environments will lead to significant changes in decomposition dynamics which cannot be captured using the current model structure.

We propose the following specific tasks for vegetation, litter and soil organic matter model parameterization and structural uncertainty investigations:

1. We will replicate the existing CLM4 litter and SOM model to represent separate but linked decomposition dynamics in the surface litter and in the mineral soil. This will allow a direct evaluation against results from the EBIS experiments and should provide a more robust framework for comparison in Year 2 against ^{14}C observations. We will also introduce a new model of fine root dynamics, which has been designed to be consistent with the proposed representation of below ground litter inputs (Gaudinski et al. in press, Gaudinski et al. 2009, Riley et al. 2009).
2. We will expand the existing ^{13}C carbon isotope capability in CLM to include also ^{14}C. This is a relatively simple model improvement that will allow a more comprehensive and direct evaluation of model results against EBIS observations, as well as an assessment of SOM turnover times in comparison to a large archive of bomb-^{14}C measurements.
3. We will expand the representation in mineral soil to include multiple layers, following the organization of layers already in place to handle soil thermal and hydrologic processes. This development will be guided in part by depth-resolved observations of temperature and moisture

response functions from laboratory incubations and field studies, currently being planned under other support, from high-latitude carbon-rich ecosystems as well as tropical and temperate sites.

4. We will introduce a mechanistic dependence of SOM turnover times on soil mineralogy and/or physical structure (aggregation, microaggregation). This will be guided in part by results from DOE-funded research activities, including EBIS-AmeriFlux and field and laboratory (including sorption, incubation, selective dissolution, and in situ characterization) studies of physical protection of soil organic matter. The new approach will relate respiration fraction and turnover times (Figure VI.1) to soil mineralogy. We will test the effects of generalization to those soil classes commonly available for global-scale modeling.

VI.2.2.2 Carbon-Nutrient Interactions

CLM was the first land model component of an atmosphere-ocean general circulation model to include coupled carbon-nutrient dynamics, demonstrating that the introduction of the concept of nutrient limitation in such a model can have dramatic consequences for all the major land-climate feedback pathways (Thornton et al. 2009). This work highlighted the uncertainty associated with current land biogeochemistry representation in climate system models, but the current representation of these dynamics in CLM is still quite simplified in comparison to the current state of knowledge as represented in some stand-alone terrestrial biogeochemistry models (e.g., Cui et al. 2005).

Known deficiencies in the current model formulation of nutrient dynamics include (1) generic representation of soil mineral nitrogen, as opposed to more realistic representation of separate NH_4 and NO_3 pools; (2) generic representation of gaseous N loss, as opposed to more realistic representation of separate N_2, NO_x, and N_2O losses; (3) simplistic representation of dissolved mineral N leaching; and (4) lack of nutrients other than nitrogen (e.g., phosphorus). CLM currently uses nitrogen as a surrogate for all nutrients, and so is certain to underestimate the influence of nutrient limitation in ecosystems where other nutrients are even more limiting than nitrogen, as is likely for phosphorus limitation in many tropical forests. Efforts are under way under other support to introduce a phosphorus component in CLM, and we expect to have this component, at least in an early prototype stage, for testing and evaluation starting in Year 2 of the project proposed here.

We propose the following specific tasks for carbon-nutrient parameterization and structural uncertainty investigations:

- We will improve parameterization of soil mineral nitrogen pools, nitrification and dentrification processes, and leaching losses to both groundwater and streamflow. We will start by using existing parameterizations from more detailed offline biogeochemistry models that include explicit representation of nitrogen transformations, loss, and plant availability (Christensen et al. 2006, Gu et al. 2009, Li et al. 1992, Maggi et al. 2008, Riley et al. 2001).
- Integrate the new mechanistic nitrogen treatment and a new phosphorus model (as available from other support) within the expanded dual-layer litter and SOM model structure emerging from Year 1 of litter and soil task described earlier.
- We will extend the representation of soil nitrogen dynamics to include reactive transport across multiple soil depths. In this effort, the new nitrogen trace gas emissions model will be implemented across multiple soil layer depths, and its performance will be evaluated and optimized against existing data sets.
- We will evaluate the use of nitrogen as a suitable surrogate for all forms of nutrient limitation by comparing nitrogen-only with joint nitrogen-phosphorus limitation in a global-scale simulation experiment. Similar experiments are included under other support, but here we will have exclusive access to the modified litter and soil model structure. We will evaluate the global-scale influence of

single and multiple nutrient limitations on land-climate feedbacks and prediction uncertainty, in the context of an optimized litter and SOM model structure.

VI.2.2.3 Prognostic Subgrid Age-Class Distributions

Disturbance history, particularly the time since last major disturbance, is known to exert a fundamental influence on net carbon exchange between land and atmosphere at any given location (Law et al. 2003, Thornton et al. 2002). CLM currently includes representation of both managed (harvest) and unmanaged (wildfire) disturbance, and also tracks the changes in land cover associated with shifting patterns of human land use. These disturbances and land use patterns are responsible for a significant fraction of the variability in net carbon exchange at the global scale on interannual, decadal, and century time scales. CLM includes a sophisticated treatment of subgrid heterogeneity that accommodates a first-order representation of these dynamics by allowing subgrid weights to shift between various plant functional types (PFT), but one major shortcoming of the current model implementation is that it does not track the subgrid distribution of time-since-major-disturbance within a given PFT. Thus, for example, a large drought that results in wide-spread wildfire might impact 50% of the evergreen forest PFT on a particular CLM gridcell, but instead of representing growth in subsequent years as intact older forest and freshly burned regenerating forest in parallel, the model merges state variables across these two distinct subsets and produces a partially reduced forest structure over the entire area that does not accurately reflect either of the observed subgrid patches.

This problem is only evident for gridcell sizes larger than the spatial scale of the typical disturbance. For gridcell resolution of 1°, typical of current operational global scale simulations, the problem could be significant. Several efforts are under way to explore this situation and to develop solutions that represent the most important dynamics of the time-since-disturbance distributions while maintaining reasonable computational costs and per-processor memory footprints.

We propose here to perform an evaluation of two such approaches, both supported under other funding, in the context of our proposed UQ and testbed/data infrastructure. The two approaches are (1) an implementation of the Ecosystem Demography model (ED) within CLM, being carried out by researchers at LANL under support from the Regional and Global Climate Modeling Program of DOE BER, and (2) an implementation using a Fixed Age Bins method (FAB), with subgrid tracking of within-bin explicit age distributions, being developed at ORNL under the Climate Change Forcing scientific focus area.

We propose the following specific tasks for age-class model evaluation to characterize land-climate feedback prediction uncertainty, and to guide model selection:

- We will perform single-factor experiments that evaluate ED-CLM vs. FAB-CLM on the basis of goodness-of-fit to forest inventory data sets compiled for North America under the land testbed/data activity (Section VI.4.6). We will generate error estimates for predicted vs observed biomass and age-class structure over forested regions of North America for the recent historical period (1980–present).
- Perform offline CLM and coupled CESM experiments to evaluate the influence of model structural difference between ED-CLM and FAB-CLM on predictions of global-scale land-climate feedback parameters. This effort will use the land UQ framework for model structural evaluation (Section VI.3.2.4). We will perform UQ analysis of propagated prediction uncertainty in feedback parameters as determined from earlier parameter sensitivity and optimization efforts and model structural differences in age-class representation.

VI.2.2.4 Prognostic Land Use and Land Cover Change

A large multi-laboratory project is under way that will deliver a new capability within CLM/CESM to predict land use and land cover change, as well as some related drivers, such as changes in energy use and energy technology, in a fully-coupled climate-integrated assessment framework. The time line for that project is such that we will have access to early prototypes as well as a final coupled model during the current proposed effort. We do not propose here to perform any additional model development on this front, but rather, we will take advantage of the land testbed/data and UQ frameworks as they mature toward the end of the project to perform a detailed evaluation of the climate feedback and prediction uncertainty consequences of this new prognostic capability.

We propose the following specific tasks for integrated CESM/GCAM evaluation to improve land-climate feedback predictions:

- We will exercise the partially coupled CLM/GCAM framework using offline forcing, first from standard reanalysis weather data and then from saved atmospheric model output, to evaluate the influence of forcing biases on prediction uncertainty. We will use the land UQ framework to evaluate prediction uncertainty for both land use/land cover predictions as well as the subset of feedback components that can be obtained from offline simulations.
- We will exercise the fully coupled CESM/GCAM framework to evaluate the influence of prognostic land use and land cover, as well as prognostic energy use and energy technology, on coupled model climate feedback parameters, using the multi-component (fully coupled) testbed/data and UQ frameworks (Section VI.4.5). We will produce UQ-derived estimates of prediction uncertainty for land use and energy components, and future changes in temperature and precipitation over land from fully coupled CESM/GCAM, and compare against results without GCAM coupling.

VI.2.2.5 Land-Climate Feedback Milestones and Deliverables

Year 1

- Implement two-layer treatment of litter/SOM pools and fluxes
- Implement and evaluate new reactive nitrogen parameterizations

Years 2–3

- Implement ^{14}C model
- Implement new nitrogen-phosphorus model
- Implement fully depth-resolved litter/SOM model
- Implement reactive transport algorithms for nitrogen in multi-layer model
- Evaluate two alternative age-class representations against inventory data

Years 4–5

- Introduce dependence of SOM model on mineralogy and physical structure
- Assess nitrogen-as-surrogate nutrient hypothesis in global model
- Evaluate influence of age-class representation on land model UQ
- Evaluate prediction uncertainty associated with forcing bias
- Evaluate coupled model prediction uncertainty associated with CESM/GCAM coupling

VI.2.3 Subgrid Land Hydrology

The terrestrial system plays an active role in the climate system through exchanges of heat, water, momentum, trace gases and aerosols with the atmosphere and also through freshwater and nutrient supply to the ocean. Based on decades of development, land models now include rather sophisticated representations of many biogeophysical, hydrological, biogeochemical, and vegetation dynamics processes. CLM has benefited from these efforts and has evolved into a sophisticated and complex model that is increasingly suited for investigations of the role of land processes in weather, climate, and climate change, including topics such as carbon and nutrient cycling, land cover and land use change, urbanization, and geoengineering as well as the study of feedbacks between the terrestrial and the broader Earth system. The increasing scope of scientific problems that CLM can be used to address requires increasingly comprehensive treatment of fundamental land processes. Soil and snow hydrologic processes are at the core of a land model, and the quality and comprehensiveness of the representation of these processes affects all aspects of the land model simulation, including those related to energy and carbon fluxes.

Although the treatment of soil and snow hydrology in CLM has advanced considerably over the last several years due to the efforts of the CESM Land Model Working Group (see e.g., Lawrence et al. 2010 and Oleson et al. 2008 for summary), the treatment of subgrid-scale variations in soil moisture and snow that exist over space scales of several to tens of meters, which has been a perpetual concern, remains unresolved. Currently in CLM, subgrid soil moisture heterogeneity is only nominally represented through a topography-based approach that links water table position to surface runoff generation. Snow heterogeneity is not treated at all. This effectively means that the highly dynamic and spatially heterogeneous hydrology is homogenized to the CLM grid scale, and as such provides highly averaged and likely biased (due to the highly nonlinear relationship between soil moisture and evapotranspiration, [ET]) values of fields such as ET, sensible heat flux, and primary productivity that drive the terrestrial water, energy, and carbon cycles. Explicit resolution of the variability in surface conditions will not be achievable for the foreseeable future. Other methods must be implemented to close the scale gap.

The treatment of rivers in CLM also requires fresh attention. Rivers integrate the signal of climate change on land and transfer this signal to oceans in the form of evolving freshwater flow volumes and nutrient loads. Although the current runoff-routing algorithm (River Transport Model [RTM]) does a credible job of representing the mean volume of runoff from the land to oceans (Branstetter 2001), it does not represent the effects of transient, seasonal and inter-annual floodplain, lake, wetland and delta inundation processes on river flow and feedbacks of these processes onto subgrid scale soil hydrology. The RTM also does not maintain a capacity to include human management of river flows through impoundments, reservoirs, or irrigation.

We identify three areas for new land hydrology model parameterization and structural uncertainty investigation that will resolve important conceptual and practical limitations to the model in its current form. We expect to be able to make robust and quantifiable improvements over the next 5 years in the following main areas:

- Improve the representation of subgrid soil water variations through adoption of a watershed-based approach,
- Represent subgrid snow depth variations via existing dynamical downscaling techniques, and,
- Adapt the RTM to permit two-way interactions between river flow and soil hydrology.

VI.2.3.1 Subgrid Soil Moisture

Subgrid scale variations in soil moisture are due to several factors including topography and its effect on lateral soil water redistribution, soil texture, vegetation, and precipitation and snowmelt distribution. One potential way to characterize the land surface is as a collection of watersheds or catchments rather than as a uniform grid of latitude and longitude. Watershed approaches are conceptually more hydrologically sound than a grid-based structure and are advantageous because they take advantage of the natural organizational structure of a landscape. Within a watershed approach, the effect of lateral redistribution of soil water on ET can be considered implicitly, as in Koster et al. (2000), by partitioning the catchment into several areas that represent distinct hydrologic regimes with differing controls on ET and gross primary productivity. The area of each regime within a watershed gridcell is a time varying function of watershed topography and bulk watershed water content. Koster et al. (2000) propose that each watershed can be partitioned into three categories representing a range of degrees of soil water saturation (e.g., upland through to wetland portions of a watershed). Sellers et al. (2007) argue that a three bin model is not able to adequately capture the nonlinear impact of soil moisture variations on ET and that 10 soil moisture bins would be a more effective level of discretization. One advantage to this approach is that it is naturally multi-scale. Watersheds can be smaller in regions of complex terrain or greater spatial heterogeneity and larger for more homogeneous subbasins. A watershed based model also enables developers and users to take advantage of nested observational data sets and will facilitate more effective use of field campaign measurement data collected at the watershed scale (e.g., long term experimental watersheds). The development of a watershed approach for CLM will also draw on techniques obtained from Hillslope River Routing (HRR), a novel multi-scale hydrologic transport model (Beighley et al. 2009). HRR is a high-resolution hydrology model that includes a detailed topographic representation of the land surface including features such as lowlands, slope, directional aspects, and a representation of wetlands, lakes and floodplains.

Although the watershed approach is conceptually more defensible than a grid-based approach, it is also considerably more complicated to implement (e.g., significant recoding of existing model tools and diagnostics), and the advantages to the watershed approach remain theoretical. It is possible that a similar soil moisture binning approach applied to a grid-based model can perform equally well to a watershed-based model. Both approaches will be implemented and tested during this project.

We propose the following specific tasks to investigate how representations of subgrid soil moisture variations influence prediction uncertainty for water and carbon fluxes:

- We will implement alternative watershed-based hydrology structure, retaining the existing parameterizations for physics within the soil-snow column.
- We will assess options for number and structure of soil moisture bins, including considerations of vertical distribution, within a watershed. We will perform a detailed assessment of the prediction uncertainty consequences of subgrid soil water discretization techniques.
- We will perform off-line CLM and coupled CESM experiments to evaluate the influence of watershed-based subgrid hydrology representation on water and carbon fluxes. We will deliver a detailed assessment of costs/benefits of watershed-based approach versus standard grid-based approach.

VI.2.3.2 Subgrid Snow Depth

Snow distributions are highly dependent on elevation. The impact of elevation on temperature, precipitation, and humidity can be captured by representing subgrid variations in surface elevation in terms of fractional area distributions of discrete elevation classes as in Ghan et al. (2002). In this scheme, for each elevation class, the downscaling scheme calculates the height of the rise or descent of air parcels traveling through the grid cell, and applies the influence to temperature and humidity profiles of the elevation class. Cloud, radiative, and surface processes are calculated separately for each elevation class. The Ghan et al. downscaling technique will be merged with Sellers et al. and Koster et al. watershed soil moisture binning technique to form a comprehensive representation of subgrid soil water and snow processes.

We propose the following specific tasks to investigate how representations of subgrid snow depth variations influence prediction uncertainty for water and energy fluxes:

- We will implement existing dynamical downscaling techniques for temperature, humidity, precipitation, and radiation and apply within multiple elevation class framework that is already used in CLM for the purpose of providing an accurate mass balance for the new ice sheet model component. The outcome will be a working subgrid snow depth distribution model.

- We will perform offline CLM and coupled CESM experiments to evaluate the influence of watershed-based subgrid snow depth representation on water and energy fluxes as well as on the timing and amount of river runoff. We will perform a detailed assessment of the costs/benefits of dynamical downscaling to multiple elevation classes approach for snow modeling vs the standard bulk approach. Emphasis will be on assessment of river runoff hydrographs and snow on and off dates in mountainous terrain, evaluated against observations (Section IV.4.6).

VI.2.3.3 River Transport Model Structural Improvements: Two-Way River-Soil Interactions

In the current CLM system, runoff that is generated at the grid cell level is sent directly to the RTM, by which it is routed through the river network to the ocean. Once the water is in a river, it no longer interacts with CLM hydrology. In reality, water in rivers can seep or flood out of rivers into the adjoining soil column when conditions dictate. Within the context of this project, the restriction of one-way water movement into the river network will be removed, and water will be permitted to enter and leave the rivers. To facilitate this two-way interaction and to aid in the computational efficiency of CLM and RTM, the RTM will be removed from CLM and implemented as a separate Earth System Model component that will interact with the rest of the system through the CESM coupler. Currently, one of the barriers to two-way CLM-RTM interactions is due to technical difficulties in mapping RTM locations back on to CLM grid cells. This limitation will be significantly eased when operating through the coupler.

The watershed approach described above will also allow a more realistic representation of the channel network compared to the eight-directional approach currently used in the RTM. The watersheds can be linked through the channel system, and runoff is routed directly from watershed to the river channel. A vector representation will be used to represent the actual channel network. A watershed approach will also ease the inclusion of human impacts such as levy building, reservoir operations, diversions, and irrigation.

We propose the following specific tasks to investigate the influence of two-way interactions between river water and soil hydrology on water and energy flux prediction uncertainty:

- We will extract the RTM from CLM and implement as a new coupled model component. We will develop new routing maps based on watershed-based grid. This effort is contingent on the prior implementation of watershed-based grid structure.
- We will improve river flow rate parameterization and develop flood parameterization. This effort will include a demonstration of the impact of two-way interactions between river flow and CLM soil hydrology with an emphasis on flood events.

VI.2.3.4 Subgrid Hydrology Milestones and Deliverables

Years 2–3

- Implement new watershed-based hydrology structure
- Evaluate options for number and structure of elevation classes
- Implement new snow depth distribution model with elevation downscaling
- Implement RTM as a separate coupled model component in CESM

Years 4–5

- Evaluate influence of subgrid hydrology structure on global water and carbon fluxes
- Evaluate influence of subgrid snow on global water and energy fluxes.
- Implement improved river flow rate and flood parameterizations

VI.3 LAND MODEL UNCERTAINTY QUANTIFICATION

VI.3.1 Land UQ Approach

The overall UQ approach as applied to the land model is to first characterize sensitivity of model predictions to variation in model parameters, then to quantify the components of prediction uncertainty associated with parameter uncertainty, structural uncertainty, and uncertainty in model forcings (e.g., surface weather), and finally, to propagate these multiple uncertainty components forward to generate an overall estimate of prediction uncertainty. This approach is implemented as an iterative process, repeated as new observational data sets and new candidate model structures are introduced. Our UQ approach produces probabilistic estimates of uncertainty in model outputs, as well as estimates of the contribution of each parameter to these uncertainties. Land UQ results will be useful in guiding subsequent observational campaigns, leading to improved estimates of parameters with maximal impact on prediction uncertainty.

Two complementary approaches will be explored for land model UQ. The primary distinction between the two approaches relates to the method of selecting optimal parameter values and assigning uncertainty estimates to these values. One approach relies on Bayesian inference to construct joint probability distribution functions (PDFs) over multiple parameters, based on a model which predicts a measured observable. The second approach uses regression methods to characterize parameter values and parameter uncertainty estimates as an optimization problem. The Bayesian inference method generates joint parameter PDFs by performing a large number of forward model evaluations for each trial set of parameter values. Optimization uses an iterative method to fit an objective function, using local calculations of first-order and sometimes second-order parameter-space gradient information. Bayesian inference and optimization methods are described in greater detail in Section VIII.3.

Because of computation time associated with a large number of forward model evaluations required by the Bayesian approach, a faster, simpler “surrogate model” must be constructed to represent the dynamics of CLM with respect to each observable of interest. Several candidate methods for constructing the land model surrogate will be explored (see Section VIII.2). The cost of building the surrogate can be reduced by using sensitivity analysis or user judgment in eliminating less influential parameters from the UQ problem. The long-term UQ text (Section VIII.2) outlines a number of global sensitivity methods that will be tested in this regard.

We will explore the use of finite difference and automatic differentiation (AD) methods to quantify local gradients in application of optimization approaches (see Section VIII.2). AD generates augmented model code which introduces new variables and calculations in all the original model algorithms to provide gradient information through application of the chain rule for partial differentiation of a complex function. Both forward mode AD (linear tangent method) and reverse mode (adjoint method) approaches will be explored.

VI.3.2 Land UQ Tasks and Deliverables

Land UQ efforts are focused on the steps necessary to arrive at model prediction uncertainty estimates and on steps necessary for propagation of multiple component model uncertainties to estimate prediction uncertainties from the fully coupled CESM. Essential components of this effort are: multivariate sensitivity analysis, parameter optimization and uncertainty estimation, evaluation of uncertainty associated with land model forcings, quantification of model structural uncertainty, and forward uncertainty propagation in the fully-coupled system. Specific land UQ tasks and deliverables for Years 1 through 5 are described in the following sections.

VI.3.2.1 Sensitivity Analysis

We will explore the use of both nonintrusive and intrusive methods for multi-variate sensitivity analysis, starting with the existing land model (CLM4). We have identified approximately 40 target model parameters over which this preliminary sensitivity analysis will be performed. Identical methods will be used to generate sensitivity analyses at multiple sites and also at the global gridded scale, but the analyses will be customized to reflect differences in observables at different scales. For example, at the site-scale we will quantify the sensitivity of carbon, water, and energy flux predictions to the target parameters at each of the eddy covariance flux sites (see data set development details in Section VI.4). At the global scale, we will quantify the sensitivity of predicted leaf area index (LAI), fraction of absorbed photosynthetically active radiation (FPAR) and similar remote-sensing observables to the same list of model parameters. This effort will result in an assessment of intrusive vs nonintrusive sensitivity analysis methods, and the generation of single-point and grid-based sensitivity analyses.

VI.3.2.2 Parameter Estimation

We will explore the use of both Bayesian inversion and optimization methods to estimate parameter values, starting with the existing land model (CLM4). Sensitivity analysis results will inform the selection of parameters to include in the estimation approaches. Parameter estimation for single-point implementations of CLM4 will be conditioned initially on carbon, water, and energy flux observations at 40 North American sites (see Section VI.4.6). Gridded parameter estimation will be conditioned initially on global-scale data sets already consolidated under C-LAMP (Randerson et al. 2009). The parameter estimation steps will be revisited periodically as new observations and new model structures are considered (as described above for specific land science investigations). This effort will result in optimized parameter estimates, including a quantification of parameter uncertainty, for both single-point and global gridded model implementations. We will prepare a manuscript describing single-point and gridded prediction uncertainties in CLM4 associated with parameter estimation.

VI.3.2.3 Forcing Uncertainty

As a critical step towards quantification of prediction uncertainty in the fully coupled CESM, we will explore the prediction uncertainty in CLM4 that is due to biased land model forcing (or boundary conditions). We will focus our efforts here primarily on surface weather forcings, including near-surface air temperature, precipitation frequency and intensity, humidity, downwelling short and long wave radiation, and wind speed. We will repeat offline CLM4 sensitivity analysis and parameter estimation performed in Years 1 and 2, replacing reanalysis surface weather forcings with equivalent output from the default CESM. We recognize numerous other forcings and boundary conditions that contribute to land model uncertainty (e.g., nitrogen deposition and soil texture), but we focus here on quantities at the interface between CLM and CAM to better inform the prediction uncertainty propagation problem for CESM. We will update previous sensitivity analysis and parameter estimation results using CLM4 and coupled model forcing for near-surface weather fields. We will prepare a manuscript describing impact of CESM climate biases on CLM4 prediction errors and uncertainty.

VI.3.2.4 Structural Uncertainty

A major concern for land model development is how, objectively, to select new development pathways from among multiple potential model structures. We have identified two fundamental land-related science questions that we think are in the critical path for a comprehensive analysis of climate prediction uncertainty (carbon-climate feedbacks, and subgrid hydrology, described above). We will use the sensitivity analysis and parameter estimation approaches refined in Years 1–3 to evaluate multiple potential model structures emerging from model development and science investigations. We approach this problem using the multimodel UQ framework described in Section VIII.3.3. Specifically, we will evaluate new vertical structure for litter and soil organic matter, new representations of nutrient dynamics, new age-class structures, new prognostic land use components, and new subgrid hydrology representations in pair-wise comparisons to CLM4. Model selection will be based on single-point and global gridded metrics (Section VI.3.2.2), and augmented at this stage in the project by additional evaluation data sets (Section VI.4.6). We will perform pair-wise evaluations of model structure, comparing results of new science developments to CLM4. This effort will include selection of preferred model structural changes and UQ iteration on the new model with merged structural changes. We will prepare a manuscript describing the impact of model development and structural change on parameter optimization and prediction uncertainty.

VI.3.2.5 Coupled Model Prediction Uncertainty

We will use forward model uncertainty propagation methods (Section VIII.3.5) to combine parameter and prediction uncertainty results emerging from land UQ efforts in Years 1–4 with similar results emerging from atmosphere and ocean/sea ice efforts. The objectives here are twofold: first, to understand how coupled system dynamics affect optimal parameter estimates and prediction uncertainty for land model observables such as single-point fluxes and gridded canopy variables; and second, to provide prediction uncertainty estimates for global-scale observables and metrics that can only be obtained from a fully coupled simulation, such as atmospheric CO_2 concentration and climate-carbon cycle feedback parameters. This effort will deliver a forward propagation of parameter and forcing uncertainty to arrive at prediction uncertainty estimates in the coupled system. We will prepare a manuscript describing the influence of coupling on land model prediction uncertainty. We will prepare a second manuscript describing the influence of land model parameter uncertainty on coupled system carbon-climate feedback uncertainty.

VI.3.2.6 Land UQ Milestones and Deliverables

Year 1

- Assessment of intrusive vs nonintrusive sensitivity analysis approaches
- Single-point and grid-based model sensitivity analyses

Years 2–3

- Optimized parameter estimates for single-point and gridded model implementations
- Updated sensitivity analysis and parameter optimization using CESM forcing

Years 4–5

- Evaluation of model structural changes, impact on land UQ
- Forward propagation of land model prediction uncertainty in fully coupled simulations

VI.4 TESTBED DEVELOPMENT AND DATA SET PREPARATION

Our vision for a land testbed is a front-end workbench oriented toward model users and evaluators. The testbed will enable direct and efficient evaluation of the impacts of changes in parameter choices or model structure; such evaluations will enable model developers or users to readily access observational data sets, and to conduct sensitivity analyses quickly and in a replicable way. Such a capability does not currently exist for CLM4. This is a serious limitation to the ability of the terrestrial modeling community to make rapid progress in terms of model development and evaluation. The development of a model testbed and associated data set preparation are the steps that allow the numerical experiments for land UQ, and eventually coupled-system UQ, to proceed efficiently and that operationalize the process of continued model improvement and evaluation.

Land components of testbed development and data set preparation efforts will proceed in parallel. For testbed development our initial efforts will focus on an evaluation of user needs, and incorporation of sensitivity analysis approaches from the UQ effort. Our initial focus for data set preparation will be on the synthesis and ingest of existing but underutilized data sets into the Earth System Grid (ESG), prioritized by the needs of early model development tasks. Subsequent testbed effort will focus on management of comprehensive sensitivity, parameter estimation, and prediction UQ workflow. An important design criterion will be to allow easy extensibility of the data infrastructure component to accommodate new observations (and new types of observations) as they become available. This capability should encourage user participation from observational and experimental communities, who would benefit from having their data available in the testbed architecture. The goal of mid-term testbed development is to have a significant amount of "push-button" capability in place, to improve efficiency of model development and evaluation through rapid and reproducible deployment of UQ methods against diverse data resources. A longer-term goal for the project is to achieve interoperability among land, atmosphere, and ocean testbeds, so that fully coupled Earth system model development and evaluation can take place within a consistent environment for workflow management, UQ methodologies, and data resourcing.

The land component of testbed development and application effort is organized around the following tasks and deliverables in the following sections.

VI.4.1 Testbed Design

Overall land testbed design criteria will be established through a series of workshops engaging Earth system modelers, observationalists, and experimentalists. Workshops for this activity (Year 1 and subsequent years) will be supported in part by the Integrated Network for Terrestrial Ecosystem Research on Feedbacks to the Atmosphere and Climate (INTERFACE) project, a National Science Foundation Research Coordination Network focused on synthesis of land experimental results and Earth system modeling (see Appendix 1, Letter of Collaboration from INTERFACE PI, Jeffrey Dukes). Land science experts will coordinate closely with the testbed infrastructure development team to provide content guidance for the testbed design phase.

VI.4.2 Testbed Support for Data Ingest/Interface

Numerical experiments described above for land UQ effort depend in part on efficient access to observational data sets. An important functionality of the land testbed will be to provide an interface to model users for ingest, display, and analysis of structurally diverse data sets. Land science experts will coordinate closely with the testbed/data infrastructure team to provide functional guidance for the data ingest and data operability development.

VI.4.3 Testbed Support for Sensitivity Analyses

Initial phase of land UQ approach is to perform comprehensive sensitivity analyses of CLM4, exploring multiple approaches. The preliminary efforts will proceed outside of the testbed, but during this exploratory phase the land science experts will be providing input to the testbed development team so that the testbed can encapsulate the necessary functionality to carry out subsequent sensitivity analysis steps. This effort will result in design criteria for sensitivity analyses, as well as a preliminary implementation using a single sensitivity analysis approach from the land UQ methods.

VI.4.4 Testbed Support for Parameter Estimation

The second phase of land UQ effort focuses on multiple approaches to parameter estimation/optimization. Preliminary efforts will proceed outside the testbed infrastructure, but these efforts will be providing design and implementation feedback to the testbed development team. The same functionality is anticipated to serve the land UQ efforts characterizing model structural uncertainty. This effort will result in a complete design for parameter estimation functionality. A preliminary implementation will be tested using single-point scale estimation at eddy covariance flux station locations.

VI.4.5 Testbed Support for Coupled Model Prediction Uncertainty Propagation

In the final phase of the land UQ effort, we will be coupling prediction uncertainties from the land model with other components to estimate coupled system prediction uncertainties using forward error propagation methods. We expect that the testbed development for land, atmosphere, and ocean/sea ice will have reached a level of maturity by the end of the project that this exercise can be conducted in a coupled testbed framework. This effort will result in a complete design for error propagation methodology encapsulated in the land testbed. This capability will also be interoperable with other component testbeds to allow prediction uncertainty estimates in CESM.

VI.4.6 Land Data Set Development

The data set development component of land data infrastructure effort consists of systematic progress through a prioritized list of existing data resources, formatting as necessary for ingest into the testbed framework, and modifying as necessary (e.g., gridding or regridding, unit conversion, metadata development/editing) to improve compatibility with CLM process-level capabilities and output structures. The diverse nature of existing data sets for land observations and experimentation makes this a challenging goal, but one which is crucial to the success of the overall goal of characterizing and reducing prediction uncertainty. Each data set presents some unique challenges, identified below, but some aspects of the effort are common to all data sets. All data sets will be converted to netCDF format, using the Climate and Forecast (CF) metadata conventions (CF-1.4, http://cf-pcmdi.llnl.gov/). We expect that some of our observational and experimental data sets will require extension of the CF conventions (e.g., new variable names, units, and data quality flags), and we will work with the CF development team at LLNL to accomplish the needed extensions. As each data set is being prepared for ingest into the data component of the land testbed, we will also query primary data providers and literature sources to generate observational uncertainty estimates, where possible. Specific land data development efforts are scheduled in each project year. Technical details for each data development task are provided below, while summary milestones for data development tasks are listed in Section IV.4.7.

VI.4.6.1 Year 1 Data Development Task Details

- Existing CLM and C-LAMP observational data sets (http://www.climatemodeling.org/c-lamp/, Randerson et al. 2009) will be brought into the ESG, and made available for test bed data infrastructure prototyping.
- Existing high-quality AmeriFlux and Fluxnet Canada observations from North American Carbon Program Site-Level Synthesis (http://nacp.ornl.gov/mast-dc/int_synth_site.shtml) will be brought into ESG, and made available for test bed prototyping. This will also provide a good prototype for resolving restrictive data-sharing policies, since these will need to be maintained as data are integrated in the test bed.
- We will initiate retrieval of global surface observations for high-resolution surface weather forcing. This will begin with ingest of Global Historical Climate Network – Daily data (GHCND), available online from the NOAA National Climate Data Center (http://www.ncdc.noaa.gov/oa/climate/ghcn-daily/).

VI.4.6.2 Year 2 Data Development Task Details

- We will continue development of high-resolution surface weather forcing data set based on GHCND, for use in testing influence of forcing bias on prediction uncertainty. This effort will require new gridding and downscaling investigations to impose high temporal frequency information from a limited number of stations on large-scale gridded data set.
- We will ingest remote-sensing observations of surface characteristics. Products from Moderate Resolution Imaging Spectroradiometer (MODIS) and Landsat imagery (and other sensors as required) will be ingested to ESG and made available through the test bed. Products will include surface reflectance, vegetation indices, FPAR, surface temperatures, and land cover characterization and land-cover change time series. Access to these products will primarily be through the Land Surface Distributed Active Archive Center (DAAC) (https://lpdaac.usgs.gov/lpdaac/), the Eros Data Center (http://eros.usgs.gov/), and the Global Land-Cover Facility (http://glcf.umiacs.umd.edu/index.shtml).

- We will expand ingest of flux observations to include ancillary site observations and a recently developed soil respiration flux database (Bond-Lamberty and Thomson 2010).
- We will ingest ARM-Carbon data sets into ESG and make them available through the land test bed data infrastructure (Fischer et al. 2007, Riley et al. 2009, Torn et al. 2010).

VI.4.6.3 Year 3 Data Development Task Details

- We will ingest nested watershed measurements from the U.S. Geological Survey (USGS) (http://nhd.usgs.gov/index.html), and ascertain the availability of similar observations from global networks. These data will be a key component of UQ for subgrid hydrology model development.
- We will ingest forest inventory biomass and age information from the U.S. Department of Agriculture (http://fia.fs.fed.us/tools-data/default.asp), and ascertain the availability of other similar data sets at global scale. This will be a key component of UQ effort to evaluate multiple age-class distribution model structures.
- We will ingest a database of depth-resolved soil organic carbon, radiocarbon, and soil N stocks, from the National Soil Carbon Network (http://forest.mtu.edu/soilcarbon/). We will also ingest existing nitrogen trace gas flux data sets (www.nrel.colostate.edu/projects/tragnet/).
- We will ingest high-resolution land cover history and disturbance data sets for North America (http://www.geog.umd.edu/nacp.goward/phase1/index.html), and ascertain the availability of similar data sets at global scale. This will be a key component of UQ efforts for age-class and prognostic land use model evaluations. The satellite period of record, particularly from Landsat and MODIS, provides a moderate-to-high resolution record of land cover history globally for the past decade, and longer in the case of Landsat.

VI.4.6.4 Year 4 Data Development Task Details

- We will ingest data from ecosystem response experiments, in collaboration with the INTERFACE Research Coordination Network (RCN) (see attached letter of collaboration from INTERFACE PI, Jeffrey Dukes).
- We will ingest a subset of over 500 newly available detailed intensive site and airborne observations from the National Ecological Observatory Network (http://www.neoninc.org/). Relevant observations include flux tower measurements, nutrient stocks and fluxes, and biometric measurements.
- We will perform a literature search and combine with remote sensing observations to derive a new data set of CLM PFTs, including new PFTs introduced during CESM/GCAM coupling.
- We will ingest data from prior intensive field campaigns (First International Satellite Land Surface Climatology Project Field Experiment, Boreal Ecosystem Atomosphere Study, and Large-Scale Biosphere-Atmosphere Experiment in Amazonia). This effort includes multi-scale (nested) measurements, and some longer-term flux tower measurements (http://daac.ornl.gov/get_data.shtml).

VI.4.6.5 Year 5 Data Development Task Details

- We will revisit previous years' data set deliverables and update with new data (e.g., new years of remote sensing inputs, new years of surface weather forcing). This is an important functionality demonstration activity for extensibility of time series information in the observations component of the test bed.

VI.4.7 Land Testbed and Data Milestones and Deliverables

Year 1

- Design criteria established for sensitivity analysis functionality
- Sensitivity analysis functionality demonstrated
- Design criteria established for land testbed data interface
- Land testbed data ingest demonstrated on C-LAMP data set
- Ingest C-LAMP data sets
- Ingest AmeriFlux and FluxNet data sets
- Initiate gridding of GHCND data set.

Years 2–3

- Design criteria established for parameter estimation functionality
- Parameter estimation functionality demonstrated with single-point simulations
- Finalize gridding of GHCND data set
- Ingest remote sensing data sets from MODIS and Landsat
- Ingest ancillary observations from flux tower locations
- Ingest ARM-Carbon data sets
- Ingest USGS watershed and river flow data sets
- Ingest forest inventory data sets
- Ingest soil C and N data sets
- Ingest high-resolution disturbance data sets

Years 4–5

- Design criteria for prediction error propagation functionality
- Land testbed interoperability with other components for coupled model error propagation
- Ingest ecosystem response experiment data sets
- Ingest NEON data sets
- Produce synthesis of PFT descriptions
- Ingest intensive field campaign data sets
- Update previously ingested data sets (as available)

VII. CROSSCUTTING ISSUES IN COMPUTATIONAL SCIENCE AND NUMERICAL METHODS

VII.1 DYNAMIC ADAPTIVE METHODS FOR ACHIEVING GLOBAL CLOUD-SYSTEM RESOLVING LENGTH SCALES

The processes governing Earth's climate system exhibit a wide range of time and space scales spanning many orders of magnitude. The multiscale nature of the scientific problem makes it extremely challenging to accurately represent all the relevant scales of motion in mathematical and numerical models, particularly with regard to treating the process of phase change, or more generally, the processes governing Earth's hydrological cycle. It is generally recognized that our ability to numerically model climate and climate change is fundamentally limited by a lack of understanding of the interaction of hydrological processes and the large-scale radiation field, particularly with respect to clouds (e.g., Stephens and Webster 1981, Cess et al. 1990). Phase transformations of water are intrinsic elements of the atmospheric circulation and take place well below the numerical truncation limit, even in the most modern of global climate system models. Clouds are a macroscale consequence of condensation processes that occur on micrometer length scales but are organized at larger length scales via a variety of complex dynamical and radiative processes, also operating over a wide range of time and space scales. The representation of clouds in global models represents a major source of uncertainty in climate change projections due to large and poorly understood feedbacks in the climate system (Dufresne and Bony 2008, IPCC 2007). Another of the key uncertainties in climate projections is how the hydrological cycle, and in particular the intensity and frequency of rainfall, will evolve in a warmer world (Allan and Soden 2008). Yet clouds, even cloud systems, and most other components of the hydrological cycle remain unresolved in current climate models and are thus highly parameterized.

While atmospheric simulations based on hydrological parameterizations have been used effectively, there are processes that are poorly represented, or not represented at all. The Intergovernmental Panel on Climate Change (IPCC) Fourth Assessment Report (AR4) (IPCC 2007) demonstrated that on global and continental scales surface temperature predictions under climate change from contemporary low-resolution (~100 km horizontal grid discretization) coupled models are more robust when compared to their performance on precipitation response (Sun et al. 2006, 2007). As horizontal length scales decrease, this discrepancy becomes worse. As stated in the AR4 technical summary, some of the key uncertainties of regional projections of future climate change were the sparse number of investigations of key components governing regional climate change, particularly with regard to the representation of extreme hydrological events, the lack of consistency in projected regional precipitation changes, and the clear inadequacy of models to properly represent the fine scales of climate response in regions with complex orography. The uncertainties associated with projecting extreme events are particularly problematical since changes in the frequency or severity of extreme weather and climate events pose some of the most significant risks to societal and environmental sustainability (Easterling et al. 2000). It can be argued that in order to attain more accurate regional projections, it is necessary to improve our understanding of the scientific reasons for inconsistencies in subcontinental projections of hydrological processes, which include model resolution (Wu and Kirtman 2007). Several recent climate studies using high-resolution atmospheric global general circulation models with resolution more typical of numerical weather prediction (Oouchi et al. 2006, Bengsston et al. 2007) have demonstrated better representations of mesoscale storm structure and intensity, even when the model fields are averaged to a coarser grid. Even large-scale phenomena, like the Southeast Asian monsoon, benefit from higher resolution (Lau and Ploshay 2009), presumably because of a more accurate treatment of individual precipitation events.

There are practical limits to the extent to which one can increase the horizontal resolution in current models. The fundamental assumption of classical parameterizations that rely on a form of statistical equilibrium begins to break down as the resolved length scales begin to approach the length scales of convective motions. This has led some investigators to explore the use of forms of cloud-system resolving models (CSRMs) for global-scale simulation problems, in which the details of the vertical dynamics and their interaction with bulk thermodynamics and phase change are resolved on the grid. For example, the "superparameterization" approach (Grabowski and Smolarkiewicz 1999, Grabowski 2001, Randall et al. 2003, Kairoutdinov and Randall 2003) employs a simplified CSRM model to replace parameterized processes. While this has shown some promising results, there are a number of issues (Randall, et al. 2003) that have yet to be resolved, such as consistency between the global scale and CSRM calculation and coupling between the two calculations, and between the noncontiguous CSRM calculations on adjacent grid cells.

A different approach, intermediate between that of superparameterization and a uniform-resolution CSRM is to employ a framework based on dynamically changing multiresolution grids. The use of variable-resolution grid systems for atmospheric modeling have been under investigation for a number of years, beginning with the work of Skamarock and Klemp (Skamarock et al. 1989, Skamarock and Klemp 1993; for reviews see Jablonowski et al. 2006, Jablonowski et al. 2009). In this approach, the fine-resolution calculation is used only in regions where it is needed, such as where the atmosphere may be undergoing strong moist convective overturning and the associated dynamical reorganization. As one of the forward-looking components of this project, we plan to develop such a model, based on the finite-volume adaptive mesh refinement (FV-AMR) approach in (Berger and Colella 1989) extended to cubed-sphere grids. This model would be, from its inception, intended to deal with dry and moist dynamics operating on a wide range of global climate time and space scales. The purpose of this model would be to provide the core computational infrastructure for the development of dynamic adaptive models at resolutions that will be feasible by the end of the decade. In the early stages of the project, we will develop a dynamical core comparable to that described in this document (Section IV.3) and couple it to Community Atmosphere Model/Community Earth System Model (CAM/CESM) physics. This will allow us to validate the overall discretization approach for climate-scale calculations, using the current physics packages in CAM. However, we emphasize that the immediate goal of this work is to develop a dynamically adaptive method to resolve time-dependent localized features in global-scale models. This is in contrast to the purpose of the local refinement capability being developed, described in Section IV.3, which provides a static refinement capability to enable more efficient model development and uncertainty quantification, that will eventually be used in a globally refined model corresponding to the finer resolution in the locally refined patch. Once we have established the efficacy of dynamic refinement on climate calculations, we will then proceed to extend the dynamical core in various ways to permit the exploration of cloud-system resolving models and potentially large-eddy simulation (LES) fluid models for dry and moist convection processes.

To carry out such a program requires a reconsideration of the representation of the fluid dynamics. The use of the hydrostatic approximation is no longer valid on the fine scales due to the large local vertical accelerations. Thus, this effort will also provide a framework for transitioning from hydrostatic to nonhydrostatic flow regimes. The existence of the atmospheric testbed under development will facilitate formal quantitative evaluations of the length scales at which the hydrostatic approximation breaks down. Therefore, in the approach taken here, we will solve the fully compressible flow equations.

VII.1.1 Basic Discretization Approach

In this finite-volume approach, the corners of the hexahedral grid are used to define control volumes, with the primary dependent variables defined as averages over the control volumes. The averages of the divergences of the fluxes that appear on the right-hand side of the dynamical equations are computed using the divergence theorem, with the integrals of the fluxes over faces replaced by some quadrature rule. This leads to a method in which primary dependent variables that satisfy conservation equations, such as total moisture and chemical species, are also conserved at the discrete level. Because of the lack of smoothness of the grid at the boundaries between coordinate patches, there is a loss of one order of accuracy in truncation error at those boundaries. For that reason, we will use higher-order (fourth-order or better) discretizations (Colella et al. 2008, Colella et al. 2010). We will combine this basic high-order finite-volume discretization method with block-structured local refinement, following the ideas in McCorquodale and Colella 2010, Zhang, Johansen, and Colella 2010. Initially, we will use the approach used in the Model for Prediction Across Scales (MPAS) and the High-Order Method Modeling Environment (HOMME) and refine only on the underlying spherical grid (i.e., use horizontal refinement). Ultimately, there are problems, such as CSRMs for stratocumulus clouds, that may require refinement in the vertical direction, a capability we will add later in the project.

Initially, we will use a semi-implicit time discretization based on the additive Runge-Kutta method (Kennedy and Carpenter 1997), but the method will be an almost explicit method: the only terms that will be treated implicitly are acoustic waves propagating vertically.

VII.1.2 Implementation Approach

The FV-AMR dynamical core will be implemented in the Chombo framework for block structured-grid methods with local refinement on high-performance computers. In Chombo, domain decomposition and message-passing interface (MPI) parallelism are built in from the very beginning, and Adaptive Mesh Refinement (AMR) calculations have been shown to scale very well for a variety of applications (Colella et al. 2007). Chombo has been under development since the late 1990s and is supported by the Applied Partial Differential Equations Center (APDEC) under Scientific Discovery through Advanced Computing (SciDAC). Over the last year, a principal goal of the Chombo team has been to develop the support required for locally refined grids in mapped-multiblock coordinates. Other applications that are using related parts of the Chombo infrastructure include the Ice Sheet Initiative for Climate Extremes (ISICLES) project, a multiresolution simulation capability for land ice in climate modeling.

Currently, parallelism in Chombo software is based on a flat single-processs, multiple data (SPMD) model, with rectangular grid patches distributed to processors in a way that minimizes interprocessor communication. This approach has been demonstrated to scale to around 16K processors and is being extended to 128K processors by reducing a major memory bottleneck (compressing the metadata that describes the distribution of patches to processors). To obtain the next increment in performance in the present context, we use a mixed parallelism model, using MPI for communication between nodes and either OpenMP, PThreads, or Compute Unified Device Architecture (CUDA)/OpenCL to implement intra-node parallel computation, depending on the architecture. This part of the work will be carried out in collaboration with APDEC project staff, who will be designing library infrastructure to hide the details of the hierarchical parallelism and architecture-dependent components from the applications-level code.

VII.1.3 Resolution Dependence of Physics Parameterizations

The parameterization challenge can be simply stated as a need to treat important motion scales below the truncation limit in a multi-scale system that does not lend itself to truncation at any particular length scale (e.g., see Figure VII.1, from Skamarock 2004). Parameterizing processes associated with phase change presents the most complex element of atmospheric modeling. Arakawa (2004) defines the problem as one of formulating the statistical effects of moist convection to obtain a closed system for predicting weather and climate. Explicitly resolved length scales for the CSSEF activity are expected to be on the order of 50 km for static global discretizations and an order of magnitude or smaller, or even less than that, for the adaptive numerical techniques that will be explored. Many of the theoretical arguments for parameterizing moist processes begin to break down at these horizontal length scales, raising questions about the viability of existing parameterization techniques at the resolutions proposed for this activity.

We recognize that errors contributed by parameterized processes may represent dominant terms in the systematic biases identified in our simulations and that these process-related biases may not necessarily decrease in magnitude with increasing resolution, in contrast to many of the errors contributed by the discretization of the dynamical equations (Collins et al. 2006). The fact that modeled features may not

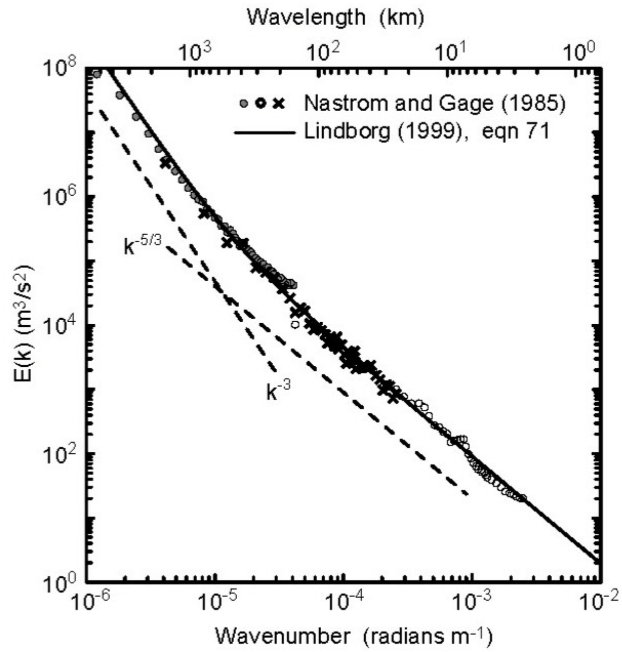

Figure VII.1. Nastrom and Gage (1985) spectrum derived from the GASP aircraft observations (symbols) and the Lindborg (1999) functional fit to the MOZAIC aircraft observations.
Source: Skamarock 2004.

converge to their observed counterparts with increasing resolution has been recognized for some time (Williamson et al. 1995, Williamson 2008) and has been observed in several different climate models (Pope and Stratton 2002). Other experiments comparing alternate parameterized formulations of convective processes in a single modeling framework have demonstrated that precipitation intensity is strongly affected by the representation of convection (Iorio et al. 2004). As discussed earlier, the vexing problem of accurately parameterizing unresolved motion scales in atmospheric models has led some to argue for brute force approaches (e.g., Randall et al. 2003), although even these proposals still do not adequately treat smaller-scale boundary layer dominated cloud scale processes (e.g., trade cumulus convection).

Based upon these investigations, we recognize that our research effort will need to include a focus on the behavior of parameterized processes at high horizontal and vertical resolution with provision for incorporating new treatments of parameterized processes, including the brute force exploration of the interaction of physical parameterizations with the underlying dynamical core.

VII.1.4 Discretization Milestones and Deliverables

By the time this project begins, we will have completed the development of the software components required to carry out this project, and have demonstrated them for two-dimensional (2D) problems (advection, shallow water equations [SWEs]) on the surface of a sphere, in joint work with Prof. C. Jablonowski of the University of Michigan and her students. We expect to continue to collaborate with Prof. Jablonowski throughout the course of this project.

Year 1

- Implementation of a verified baseline version of FV-AMR, based on the flat parallelism model.

Year 2

- Coupling of the new dynamical core to CESM. Testing and validation against HOMME multiresolution hydrostatic dynamical core at resolutions where both are expected to be valid.

Year 3

- Implementation of hybrid parallelism in new dynamical core, and baseline measurements of performance.
- Begin investigation of physics parameterizations for dynamically-refined grids, with particular emphasis on finest scales at or below 3 km mesh spacing. This work will be done in collaboration with the test bed, UQ teams.

Year 4

- Complete implementation of hybrid parallelism in FV-AMR, and demonstrate that it runs at scale on at least one of the next-generation LCF systems.
- Extension of FV-AMR to permit vertical refinement. This capability will enable LES simulations of stratocumulus clouds.

Year 5

- Continue work on new multiresolution physics models, with CSRM of tropical convective storms and tropical cyclones as the target science applications.
- Delivery of a version of FV-AMR that runs at scale on the second LCF system.

VII.2 CROSSCUTTING CHALLENGES IN COMPUTER AND COMPUTATIONAL SCIENCE

The current class of petascale computer systems frequently exhibits a large gap between peak theoretical capabilities and the level of performance realized by state of the art large-scale global climate modeling applications. Climate modeling is not unlike many other intricate multi-scale multi-physics simulation applications that are challenged to extract a large fraction of the potential performance of these complex computer systems. Indeed, over the next decade, extreme-scale computer systems will present new challenges to application development that will likely widen existing performance gaps, preventing the productive use of these systems.

The broader community consensus is that there is considerable potential to rethink both algorithm and software design in order to better exploit the hardware performance capabilities already present in the petascale systems of today and the heterogeneous multi-core systems that are expected to materialize over the next 5 years. New challenges will arise due to the emergence of hybrid processor architectures, the need to exploit higher levels of asynchronous parallelism, decreasing memory bandwidth and increasing latency in a more complex hierarchy of memory systems, and the need for application resilience because of the potential for increasing system fault rates. Solutions to realizing the full potential of future generations of extreme-scale computing systems need to involve the design and development of appropriately balanced hardware, system software, advanced programming languages and environments, architecture-aware numerical methods, and algorithms that more naturally express parallelism and data locality, all driven by new and innovative formulations of the basic application problem. It is not within the scope of this activity to take on the broader computer architecture and computer science elements of a comprehensive effort to enable the successful deployment of extreme-scale computer systems. However, the climate modeling community must maintain a tight partnership with these broader community efforts, particularly through its own focused efforts on innovative, collaborative research in applied mathematics and computer science.

VII.2.1 Scalability, Resilience and Data Locality and Migration Challenges

With the plateau in processor clock speed and the associated slowdown in thread speeds, scalability has become the most important performance element in the implementation of scientific applications on the latest generation of high-performance architectures. Computational performance is now largely a function of the ability to efficiently exploit large numbers of processing cores, numbers that have recently grown at an exponential rate. The application scientist must identify new sources of parallelism and find ways to implement code to manage hundreds of thousands of threads today, which will become millions over the next few years and billions of threads by the end of the decade. As leadership-class systems continue to scale in complexity, it is widely recognized that resilient frameworks must be fully integrated in the programming and communication model to effectively utilize them. There is also the acknowledgement that without a scheme to orchestrate data dependent tasks for data analysis and to manage the data produced by the simulations, there is no value in accelerating the computation. The end-to-end solution must be considered, or scalability will be limited by the ignored bottleneck(s).

VII.2.2 Scaling to Millions of Processors

State of the art global climate system models in 5 years, using standard domain decompositions, will permit at most several hundred thousand processor cores. Achieving greater scalability for a fixed problem size will depend on new algorithms and new ways to exploit parallelism at a finer grain than domain decomposition allows. These tasks will fundamentally include the investigation of algorithms and data representations that minimize data movement in the context of scalable multiresolution decompositions. A part of the scalability challenge will require that the simulation enterprise be nimble with regard to the programming model. As the de facto standard for high-performance computing for more than a decade, MPI has provided the mechanisms for needed scaling and performance on distributed memory systems. However, MPI has limitations that can inhibit application performance on large-scale machines containing heterogeneous multi-core processors, including limitations associated with processes that require the copying of data and a "flat" architectural paradigm (i.e., all of the processes that encompass a parallel application are assumed to be equidistant from each other with no acknowledgement of the inherent hierarchy in the memory subsystem or in the communication network). To increase scalability, the modeling activity will need to explore future and evolving parallel programming constructs such as architecture-aware hierarchical implementations of MPI. As one example, a hierarchical MPI is an attractive approach since it will not require the rewrite of codes in a totally new programming model, and shared-memory parallel programming can be exploited using simple control structures to make work and data sharing straightforward. Techniques for the exploitation of parallelism within nodes (i.e., new shared memory runtime paradigms) are also under development and will need to be leveraged to take full advantage of new architectures.

VII.2.3 Resilience of Petascale to Extreme Scale Computational Implementations

Resilience is a measure of the ability of a computing system and its applications to continue working in the presence of system degradations and failures. The resilience of scientific applications must now include the notion of continuous execution despite detectable but uncorrectable errors in the underlying computer system hardware and software stack. Studies have shown that failures will become so systemic that improving resilience at performance levels beyond the petascale will not only be imperative, but will require a more holistic approach to the detection and recovery from faults, allowing all the parts of the system to adapt to changes in the computational infrastructure. The CSSEF computational implementation will need to leverage developments in fault-tolerant MPI routines and programming paradigms to allow continuous execution of climate simulations in the presence of system faults at the extreme scale. As the scale and complexity of computer systems and climate simulations grow, it will be increasingly important to validate new system algorithms that are not corrupted by numerical instability or errors from an accumulation of transient nonfatal faults. This will include the ability to validate scalable, high-performance run-time frameworks that can reconfigure task workflows at execution time to handle faults and other changes in the runtime environment. These new environments will likely include new types of data structures, methods for exploiting the potential for recomputation rather than replication, and the incorporation of techniques with potential to replace lost data. Implementation and testing of these resiliency measures will need to be approached systematically, starting with the development of unit-testing methodologies. Continuing execution after taking the appropriate action, dropping a node or recomputing a result, will be the metric of success.

VII.2.4 Parallel I/O

Advances in observational and computational technologies have led to an exponential growth in the volume, variety, and complexity of scientific data, resulting in a growing number of petabyte-scale and soon exabyte-scale archives. Leading examples include climate simulations which are expected to generate data of significantly great size over the next few years (DOE 2008). However, data movement and input/output (I/O) performance in particular, have been the limiting factor for climate simulations for quite some time (Kleese 1999, Steenman-Clark 1999). A general, scalable solution for effective parallel I/O from high-resolution climate model simulations continues to elude systems and application programmers. The core underlying reasons include deep memory hierarchies, relatively slow external disk systems, multiple layers of control and coordination required in the system software stack, and abstractions that hinder optimization and scalability.

Traditional approaches of sequential simulation and analysis steps as well checkpoint/restart will no longer be tractable approaches at the extreme scale. Analysis data sets will present the biggest challenge in both the near term and as computational frameworks move toward next-generation system architectures. The climate application community will need to exploit new base technologies and the associated applications and libraries in order to include parallel I/O and data analysis capabilities that will be supported by future hardware technologies. We note that the broader adoption of new approaches to managing data will impact work on mathematical algorithms, data-layout for parallelization, and analysis algorithm design. Current state of the art climate simulation data analysis utilizes uniform spatial and temporal output via the parallel I/O stack into history files. As climate simulations transition to high-resolution both spatially and temporally, the number of files generated for a single climate run and the number of elements within each file will quickly overwhelm the capabilities of current generation parallel I/O environments. Complicating matters further is the fixed resolution of today's models in which the highest resolution required for subsequent data-analysis has generally been output globally, requiring data-analysis tasks to sift through tens of thousands of files to extract features of interest for further examination. This data analysis may run for hours at low and medium resolution but would require days or even weeks of execution for comparable analysis of high-resolution data sets. Continued use of these techniques is not tractable at the extreme scale. The report on the Mathematics for Analysis of Petascale Data Workshop states: "According to climate scientists there already is too much data to analyze, and in many cases the analysis of the data is more complex and takes more time to run than the original simulation" (Kegelmeyer 2008).

To address these issues, the CSSEF project will need to adopt fundamental shifts in current approaches to managing data. Embracing new data models will preserve features of interest at the temporal and spatial frequency required for further analysis tasks while substantially decreasing the storage and data movement requirements for post analysis. Such data models will also be designed to map well to next-generation storage systems that will be increasingly hierarchical and topologically dispersed within extreme-scale systems (Kogge 2008). This type of data model will map well to simulation approaches like the adaptive mesh refinement techniques discussed earlier.

VII.3 SOFTWARE COUPLING FRAMEWORKS

Earth system models are, and will continue to be, implemented by coupling separate component models via a coupling interface. Each subsystem model employs discretization approximations appropriate to its required fidelity. The challenge of implementing coupling mechanisms in parallel environments is called the "parallel coupling problem" (Larson 2009). Key resource-intensive operations include intermesh interpolation of field data; parallel transfer of data between subsystems, also called the M x N problem (Bertrand et al. 2006); time averaging and accumulation of state and flux data; and merging of output fields from multiple subsystems for input into another subsystem.

Future science goals in the proposed project's timeframe and scope include support for high- and variable-resolution meshes, support for diverse new spatial discretizations, volumetric coupling of regionally refined circulation models to the global system, and data assimilation.

VII.3.1 Growing Computational and Performance Requirements

CESM's current coupling infrastructure, CPL7, is based on the Model Coupling Toolkit (MCT) (Larson et al. 2005, Jacob et al. 2005). At present, CESM scales to tens of thousands of cores, but has likely reached its scaling limit. MCT relies on copying of subsystems' field and flux data into its own custom data structures, and MCT achieves high-speed data transfers by replicating domain-decomposition descriptors, which enables embarrassingly parallel computation of communications schedules for M x N transfers. These aspects of CPL7/MCT allowed a simple, scientific-programmer-friendly interface, but are unlikely to scale to next-generation systems. Furthermore, next generation climate model coupling infrastructures must support multiple levels of parallelism. At present, CPL7 is solely MPI-parallel and MCT makes limited use of OpenMP.

In this project's timescale, CCSM4/CESM1 must be enhanced so it can scale to new hardware and a new coupling infrastructure capable of supporting future versions of CESM outlined in its 2011-16 science plan (CESM SSC 2009). Key requirements include: support for multiple levels of parallelism and accelerator technologies such as graphics processing units (GPUs); the ability to handle a wide variety of structured and unstructured meshes found in new model formulations; scalable run-time support for computation of intermesh transformation coefficients; and support for multiple levels of process composition to optimize usage of ultrascale process pools.

VII.3.2 Foundations for Future Coupling Strategies and Path Forward

While MCT performs most of the runtime coupling functions in CESM, the calculation of interpolation weights is performed offline. The Spherical Coordinate Remapping and Interpolation Package (SCRIP) was released in 1998 and was developed for interpolation of field data between any two horizontal grids on the surface of a sphere. SCRIP supports nearest-neighbor distance-weighted averages, bilinear, bicubic and first- and second-order conservative remapping schemes (Jones 1999). SCRIP's weaknesses are (1) the methods used to generate the weights currently are not very robust near the spherical polar singularities, and (2) the lack of assumptions about the underlying grid hamper optimization and prevent use of monotone limiting for higher-order interpolations that require gradient computations.

We will address limitations in MCT and SCRIP for this project by building new versions based on the Mesh-Oriented datABase (MOAB) package. MOAB is a library for representing grids and solution fields associated with grid entities andhas already been implemented and demonstrated as part of the Nuclear Energy Advanced Modeling and Simulation (NEAMS) program (Tautges 2009). MOAB represents a full range of grid types, including structured, unstructured finite element, and polyhedral grids. MOAB includes a full domain decomposition-based parallel model, providing information about grid entities shared between processors and representing an arbitrary number of layers of ghost entities from neighboring processors. Various simulation services already interfaced with MOAB include parallel partitioning, based on the Zoltan partitioning library (Devine 2002); visualization using the VisIt tool (VisIt 2005); and mesh generation using a variety of meshing tools, including CUBIT (Sjaardema 1994) and MeshKit (MeshKit 2010). We will implement SCRIP and MCT coupling methods in a MOAB-based framework, and develop interfaces to that coupling functionality for CESM. MCT's design philosophy will be retained as we will use MOAB's classes and methods corresponding to MCT counterparts, while providing an interface that will look largely identical to MCT/CPL7. This will result in new and dramatically more powerful MOAB-based versions of MCT and the CESM CPL toolkit. Once a new, MOAB-based coupling data model is implemented, MOAB's interpolation functionality will be exploited to provide more complete and sophisticated services for spatial interpolation and enforcement of conservation of interpolated fluxes. Both linear and nonlinear transformations will be supported along with interpolation of vector fields.

Once the new generic coupling infrastructure is complete, the CPL toolkit and coupler application will be reimplemented. The new CPL toolkit code base will be simpler (as it will then get its current classes from the MOAB-based MCT), and considerably more powerful and flexible. The infrastructure on which the CPL toolkit depends will offer a multilingual application program interface (API), allowing more rapid prototyping of coupled system application in high-level languages, and will make more feasible earlier work in prototyping a Python CCSM3 coupler (Tobis et al. 2010). Numerous improvements to SCRIP will also be developed, including, more robust algorithms, improved higher-order interpolations and monotone limiting, regridding and interpolation of vector fields, parallel regridding, on-line computation of regridding weights, and optimized performance.

VII.3.3 Coupler Development Milestones and Deliverables

Year 1

Implementation of MCT Data Model using MOAB classes, with MCT test cases prototyped Increase robustness of current SCRIP Package

Year 3

Complete MCT implementation based on MOAB classes and methods. New prototype CPL toolkit embodying new MOAB-MCT implementation working with "data" models MOAB-based implementation of SCRIP Improved higher-order interpolation methods

Year 5

Complete coupling infrastructure running at scale parallel, online computation of interpolation weights for a wide variety of model meshes Regridding of vector fields across singularities and on naïve staggered grids

VII.4 COMPUTATIONAL RESOURCE REQUIREMENTS

Access to significant high-performance computational resources will be essential to the scientific and technical success of this project. The resourcing requirements will grow over time, where precise estimates of the project needs will have to be updated as the CSSEF team builds familiarity with the different simulation and analysis tools that will be developed over the initial five year period of performance. Some of the more difficult tasks to estimate are associated with the uncertainty quantification components of this work, where things like optimal ensemble size and optimal component model configurations still need to be explored. Analysis of year one tasks suggests that an allocation of 150M processor hours (equivalent hours on the Jaguar OLCF computer system) will be required. This requirement will grow by at least an order of magnitude as the simulation enterprise achieves goals associated with the deployment of a 1/8° global Earth System Modeling system and the attendant UQ and test bed components.

The growth in resource requirements is consistent with the planned growth in computational capability at the Office of Science ASCR Leadership Computing Facilities. We intend to exploit the ASCR Leadership Computing Challenge (ALCC) Program, designed to provide support for *high-payoff simulations in areas directly related to the Department's energy mission in areas such as advancing the clean energy agenda and understanding the Earth's climate*, as a vehicle for providing the required levels of computational support at the Argonne and Oak Ridge Leadership Computing Facilities. Despite the anticipated magnitude of a request to support the early stages of the CSSEF activity, it should still fit well within currently available resources.

VIII. CROSSCUTTING AND LONG-TERM RESEARCH IN UNCERTAINTY QUANTIFICATION

VIII.1 OVERVIEW

The proposed crosscutting and long-term research in uncertainty quantification (UQ) activity has two main goals:

- Integrate the various UQ activities in the atmosphere, ocean, and land components; and
- Make progress toward UQ of the fully coupled Community Earth System Model (CESM).

The specific UQ tasks within the atmosphere, ocean, and land components are targeted at improving and characterizing the predictive fidelity of the components. Although very different in focus, the component-specific UQ tasks share many common UQ techniques (e.g., parameter calibration). The first goal aims at integrating some of the UQ activities at the component level in order to draw on a common pool of UQ expertise and methods. The second goal, aiming for a UQ of the fully coupled system, which one can argue is the ultimate goal, is a complement to the bottom-up approach at the components level.

The main tasks of the crosscutting and long-term UQ efforts are therefore:

- Adapt and advance the core crosscutting climate UQ methodologies that support the UQ activities in the CESM components and the long-term climate UQ needs of CSSEF, and
- Advance the state of climate UQ to meet the complexity of future CESMs, observational data, and computer platforms.

VIII.2 CROSSCUTTING UQ ACTIVITIES AND METHODS

The proposed UQ tasks outlined previously in the atmosphere, land, and ocean components of the CESM all rely on a core set of crosscutting UQ activities and methods. The crosscutting activities include the application of a broad suite of UQ methods relevant to CSSEF, including methods for sensitivity analysis, the construction of surrogate models and response surfaces, input parameter calibration studies, the forward propagation of uncertainties, and an assessment of model discrepancies and structural uncertainties. Figure VIII.1 summarizes the broad UQ activities as they relate to the science goals of the CESM components. For example, the UQ tasks in all three components call for sensitivity analysis and model calibration.

We provide here a brief introduction to the crosscutting UQ activities that will be applied to the CESM. Further descriptions of the activities and methods are given in the *UQ Methodology* appendix to this document. Even though these UQ activities and methods have been applied to many different types of complex simulation models, including climate models, considerable effort is still required to apply them to the CESM and observations.

We have broadly identified the following four climate UQ crosscutting activities relevant to the CESM:

1. *Sensitivity Analysis*. Methods to analyze the local and global response and sensitivity of climate quantities of interest (QOIs) with respect to uncertain input parameters. One important example is the sensitivity of the rate of precipitation to convective entrainment. Another example is illustrated in Figure VIII.2. Sensitivity analysis is used to rank and screen uncertain input parameters in terms of their influence.

	Sensitivities & Uncertainties	Observations & Calibration	Model Development
Land	• About 40 parameters (6-12 main drivers) • Forcing from CAM ensembles	• FluxNet data at sites • Global gridded data • Multi-site calibration (real and 'proxy' sites) • Global calibration	• Ecosystem demography • Soil carbon dynamics • Subgrid scale hydrology
Ocean	• Eddy mixing in Gent-McWilliams scheme • Resolution of static refined meshes	• T, S, ACC transport, CFC ventilation • Calibrate kappa-i as a function of (x,y,z)	Optimal placement of high resolution meshes using calibrated eddy mixing
Atmosphere	• About 20-30 parameters (cloud formation, convection, etc)	• ARM data at individual sites • Calibration at sites using statically refined mesh	New parameterizations of convection and cloud processes

Baseline assessment → Optimized models → Model improvements

Figure VIII.1. Crosscutting UQ activities applied to the CESM component models. For example, sensitivity analysis and parameter calibration exercises will be applied to each component.

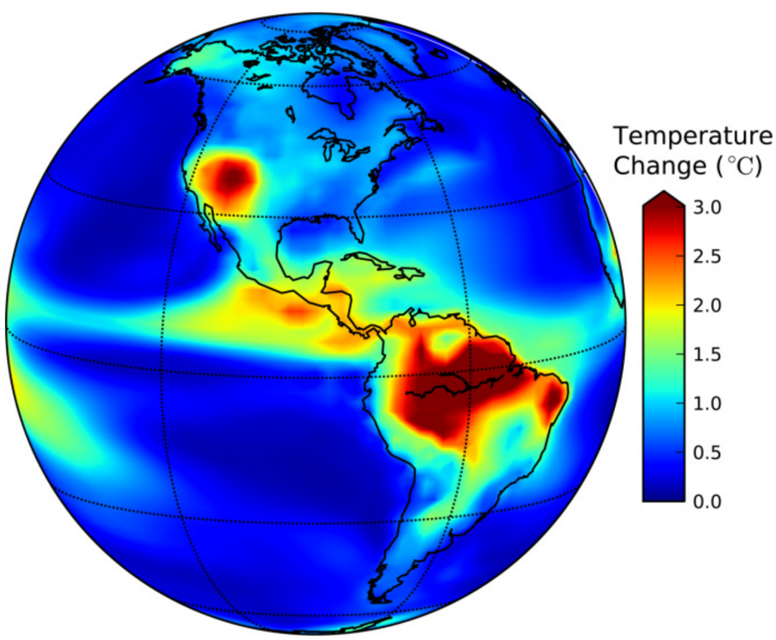

Figure VIII.2. Magnitude of the sensitivity of surface temperature in CAM3.6 to changes in the timescale parameter *tau* in the Zhang-McFarlane convection scheme. The sensitivities are global sensitivities in a 21-dimensional parameter space (figure from "Narrowing Uncertainties," Science and Technology Review, 2010).

2. *Surrogate Models*. The quantities of interest from CESM simulations will include spatiotemporal summary statistics across multiple output variables. Given the computational expense of CESM simulations at a fixed set of input parameters, there is clear value in building accurate surrogate models (also called meta-models, emulators, or statistical response models) that represent the relationships between the input parameter and the QOIs. Such surrogates can then be queried extensively for both forward and inverse UQ, detailed sensitivity analysis, or for optimization purposes. Multiple types of surrogate models appropriate for the CESM components will be developed.
3. *Model Calibration*. Methods for statistical calibration and tuning of uncertain input parameters given sets of climate observations. This activity, which is also referred to as *inverse UQ*, includes methods that account for observation and structural errors. The CESM land and atmosphere components, for example, will be calibrated using observations from the AmeriFlux network and Atmospheric Research Measurement (ARM) sites, respectively.
4. *Forward UQ*. Methods to characterize and validate the predictive accuracy of a climate QOI by propagating input uncertainties through the calibrated CESM components. This activity will also account for additional structural error and will provide methods to validate the predictions and to properly select predictions from competing models.

Multiple methods will be implemented and tested for each task (e.g., for input parameter calibration) to determine robustness and to characterize the pros and cons of each method. The UQ activities will initially use standard, established nonintrusive UQ methods. These methods treat the climate model as a "black box" that is executed at selected input configurations, yielding an ensemble of climate simulations.

VIII.2.1 Sensitivity Analysis

Sensitivity analysis methods are used to identify "influential" uncertain input variables (Saltelli et al. 2001). This information is useful for understanding CESM responses and for reducing the dimensionality of the input parameter space for UQ studies and developing surrogate models. Nonintrusive sensitivity analysis methods broadly fall into two categories: those that interact directly with the model and those that use fast statistical output emulators. The first class of methods is driven by direct input sampling schemes that are computationally efficient in estimating sensitivity indices (e.g., Morris 1991). The second class of methods is driven by (often adaptive) sampling schemes that produce accurate output statistical emulators, which can then be efficiently sampled as many times as needed to yield sensitivity indices (e.g., Oakley and O'Hagan 2004, Storlie et al. 2009, Sudret 2008, Gramacy and Lee 2008, Tang 2010). Further, the surrogate models can be used in place of expensive CESM simulations for exploratory and statistical analysis of climate QOIs. For components or specific processes of the CESM, intrusive automatic differentiation offers the capability of efficient computation of local sensitivity information, which is particularly efficient for high-dimensional input spaces.

VIII.2.2 Surrogate Models

Given the computational expense of a single CESM simulation at a fixed set of input parameters, there is clear value in building accurate surrogate models (also called meta-models, emulators, or statistical response models) that represent the dependence between input parameters and QOIs. Such surrogates can then be queried extensively for both forward and inverse UQ, detailed sensitivity analysis, or for optimization purposes. As the surrogate model is just an approximation to the actual CESM, uncertainty in the estimation of the surrogate has to be accounted for in the downstream UQ analysis. The goal is to develop and explore multiple types of surrogate models. Specifically, we will focus on three classes of surrogates: *spline-based methods* (e.g., Multivariate Adaptive Regression Splines [MARS] [Freidman 1991]); *stochastic expansion methods* that employ orthogonal polynomial representations of a QOI over the input parameter space (e.g., Polynomial Chaos expansions and stochastic collocation [Ganhem and

Spanos 1991]); and *Gaussian process models* that are based on spatial statistics, with the idea that points close together in input space should have responses that are correlated (e.g., Sacks et al. 1989, O'Hagan et al. 1999, Rasmussen and Williams 2006, Santner et al. 2003, Gramacy and Lee 2008).

We will also explore methods that can produce reduced order models for the response process (e.g., Karhunen-Loeve and expansions [Karhunen 1946, Loeve 1955]) that represent a stochastic process as a linear combination of a countable number of uncorrelated random variables (Higdon et al. 2008).

VIII.2.3 Model Calibration

Multiple methods are available for parameter calibration, including Bayesian inversion, which yields a posterior probability distribution function (PDF) of uncertain input parameters (e.g., Kaipio and Somersalo 2005, Tarantola 2004). The targeted calibration methods for the CESM components need to handle high-dimensional uncertainty input spaces and to take advantage of multiple, heterogeneous datasets whose accuracy is often not well characterized. For an accurate input calibration, it is important to account for unexplained model discrepancy (structural error) in the calibration process. As in the case of emulator-based sensitivity analysis, most calibration methods rely on statistical emulators (such as Gaussian process models and Polynomial Chaos expansions) that are trained on a carefully crafted ensemble of simulations, which often need to be designed adaptively, with feedback from the calibration process. For the CESM land component, an intrusive model calibration approaches that takes advantage of automatic differentiation will be applied. This technique offers the promise of breaking the barrier of very large data sets and large dimensional parameter spaces.

VIII.2.4 Forward UQ

There are various methods available for the forward propagation of input uncertainty. The targeted methods for CSSEF will rely on sampling techniques to generate an ensemble of simulations used to train statistical emulators, as in the case of sensitivity analysis and calibration, to yield efficient propagation of uncertainty. The emerging issues are how to effectively construct the ensemble, and how to deal with high dimensional input and output spaces. Some examples of forward uncertainty propagation for the CESM components include:

- *Atmosphere*–propagate uncertainties in convective and cloud process parameterizations to surface temperature, relative humidity, and precipitation rates;
- *Land*–propagate uncertainties in vegetation physiology, soil organic matter depth distributions, sub-grid soil moisture, snow distributions, and atmospheric forcing to surface carbon, water and energy fluxes; and
- *Ocean*–propagate uncertainties eddy mixing coefficients to temperature and salinity.

Note that a critical part of forward UQ will be identifying the structural error associated with the model and including that in the forward propagation along with the parameter uncertainty.

VIII.2.5 Future UQ Methods

While the core methodologies will meet most of the CSSEF UQ needs, some specific challenges exist, especially in scalability of the methods. These challenges, such as massive multi-scale datasets, the growing collection of uncertain model parameters, and computational complexity of the models, will require the development of novel tools. Various approaches such as advancing adaptive sampling and surrogate modeling for large I/O spaces, scalable methods for high-resolution spatio-temporal uncertainty, high-dimensional optimization and Bayesian inversion methods, and reduced-order, low-fidelity models will be pursued and promising candidates will be further developed and added to the set of methods as they mature.

The *UQ Methodology* appendix to this document contains further descriptions of core CESM UQ methods.

VIII.3 ADVANCING UQ FOR CESM

While the core crosscutting UQ methods have proven useful and effective in a number of climate UQ studies and related applications, it is not clear that such approaches, on their own, will be sufficient to deal with UQ challenges posed by future generations of the CESM. Even with advances in computing power, the added complexity of CESM may render current UQ approaches based on large ensembles of both uncoupled CESM components and fully coupled CESM infeasible. For example, the atmosphere test bed activities call for both sensitivity analysis and calibration of a relatively large collection of targeted uncertain parameters, which will require hundreds (potentially thousands) of climate simulations using the traditional sample-based UQ framework. This is achievable now with static mesh-refinement at selected sites and by carrying out Community Atmosphere Model (CAM) runs over a relatively short time period (2–3 years). However, this approach will be problematic for more complex CAM runs operating at finer (global) resolution over a longer time period.

We propose to tackle this issue by advancing existing UQ methods and by developing new UQ algorithms and approaches that will be tailored to the next-generation CESM computing architecture and data sources. While some novel methodological advances may be required, the majority of this work will be based on tailoring known methods and approaches to leverage available resources and to make use of modeling insights to develop more-efficient approaches for quantifying uncertainties. In particular, we plan to exploit our relationship with modelers and high-performance computing (HPC) experts so that we can develop new UQ approaches that go beyond treating the CESM components and computing architectures as black boxes (i.e., nonintrusive methods).

The advanced UQ efforts are binned into the following research areas: advancing nonintrusive UQ methods for CESM, intrusive methods more suitable for next generations of computer platforms and CESM versions, model UQ, UQ for large datasets and data streams, and UQ of coupled CSEM. Each research area is focused on a particular strategy for improving efficiency in UQ for the next generation of CESMs or data sources. Each of these research areas carries some risk, but there is little or no dependency across thrusts; success in one of these research areas will improve UQ efficiency, regardless of what happens in another.

VIII.3.1 Efficient and Adaptive Non-intrusive UQ for CESM

The starting points for UQ of the CESM are relatively well established nonintrusive UQ methods that were briefly reviewed in Section VIII.2 and were extensively referred to in the UQ activities in the atmosphere, ocean, and land component Chapters. However, applying these methods to a complex system like the CESM, either to an individual component (in particular CAM) or to the fully coupled system, will pose significant challenges that need to be resolved.

VIII.3.1.1 Sampling high-dimensional uncertain input spaces

Adaptive methods to sample a *high-dimensional* collection of uncertain inputs are critical to the nonintrusive UQ methods that will be applied to CESM and its components, because of the computational cost of each simulation (the CAM sensitivity/calibration/validation platform is particularly relevant in this context). We propose to advance methods that adaptively construct an ensemble of simulations by taking an initial set of sample points and then augment the initial set of runs with a sequence of additional runs, with each determined by feedback from previous simulations. One family of such adaptive sampling methods is driven by feedback from the surrogate model that is at the core of the sensitivity and calibration methods applied to CAM and the Community Land Model (CLM). These methods usually work by adaptively choosing sample points for maximal efficiency, according to some improvement criterion, for example, to maximize global prediction accuracy (e.g., Gramacy and Lee 2009) or to determine a given level set (e.g., Bichon et al. 2008). Another family of methods is based on importance sampling criterion, which sample random variables, focused on "important" values of the input variables to improve the estimation of a statistical response of interest (West and Swiler 2010). In addition to efficient sampling schemes for sensitivity and calibration, advances have to be made to forward a UQ sampling scheme in high dimensions. Promising approaches include reduced order approximations to capture the most relevant dimensions or manifolds in the input space. For example, High Dimensional Model Representation (HDMR) effectively decomposes smooth functions of multiple parameters into sums of simpler, lower-dimensional functions (Rabitz and Alis 1999, Ma and Zabaras 2010) and the Proper Generalized Decomposition (PGD) using combination of low-rank components (Nouy 2007).

We will use adaptive sampling methods in the atmosphere UQ testbed (Section IV.4) to construct informative ensembles of CAM simulations for sensitivity studies and calibration (both for the initial single-resolution sensitivity test platform and in particular for calibration of the static mesh-refined CAM) and for forward UQ for model validation. Similarly, we will use adaptive sampling to train accurate surrogate models in the global-scale sensitivity and calibration of CLM experiment (Section VI.3).

VIII.3.1.2 Efficient statistical emulators for multivariate high-dimensional CESM output

As reviewed previously, surrogate models (statistical emulators) play a significant role in nonintrusive sensitivity analysis, calibration, and forward uncertainty propagation across the various CESM UQ activities. Even though surrogate models have a long history in UQ, the use of surrogate models in CESM UQ analysis will face some challenges, namely large uncertain input space and typically multivariate output space. This applies particularly to the proposed UQ activities for CAM and CLM, both with considerable large collections of uncertain input parameters and output of interest that spans multiple output variables, with each output variable consisting of various summary statistics (metrics) describing complex space-time fields.

We plan to advance surrogate-based UQ analysis for CESM to better cope with (1) large uncertain input spaces, (2) high-dimensional output fields, and (3) multiple output variables. We plan to investigate and expand on current approaches based on reduced representation using basis functions, for example the Karhunen-Loeve (KL) representation (Higdon et al. 2008) and other similar sparse (stochastic) representations of the surrogate model.

VIII.3.1.3 Developing resolution-aware parameterizations

If the Model for Prediction Across Scales (MPAS) dynamical core gains acceptance, then we can expect to work on static (but variable-resolution) grids. It is expected that parameterizations of subscale phenomena (e.g., Gent-McWilliams and LANS α for ocean modeling) will likely depend on the local grid resolution. Hence, we anticipate the need to develop parameterizations of these models that depend on the local resolution of the MPAS grid. We expect to be able to develop these spatially varying parameterizations using information from numerical experiments as well as from calibration to physical observations such as eddy formation and temperature-depth profiles.

VIII.3.2 Tailoring UQ to High-Performance Computing and Computational Models

To be able to scale on hybrid and massive exascale platforms, UQ methods will also need to evolve to exploit the new computing resources and the structure within the computational models for the next-generation CESM. In addition, next-generation CESM components, such as land and ice sheets, will likely require highly parameterized model descriptions that will be problematic for most current UQ approaches. UQ will take a similar path in order to cope with the massive amount of streaming data that cannot be archived for post-analysis. The next-generation CESM will pose new challenges. Compared to most mature approaches, model embedded (intrusive) UQ methods will reside closer to the simulations both methodologically and architecturally to be highly parallel and compatible with the targeted hybrid exascale systems.

VIII.3.2.1 Scalable optimization and estimation for highly parameterized models

For CESM components, particularly land surface models, numerical optimization is an important technique to fit high variability models (Section VI.3). Nevertheless, future models face several challenges, such as extremely large data sets, increased dimensionality of the parameter space, and complex relationships between variables (such as dynamical dependence) and constraints (such as stability constraints). To address these challenges, we will develop scalable optimization methods for fitting complex CESM components, using the land surface models for the initial application. To compute the gradients of the objective function and the constraints, we will use recent advances in automatic differentiation (AD) and/or adjoint modeling. Scalability of the resulting optimization algorithm will be achieved by exploiting the derivative information calculation for fixed parameter values (which is embarrassingly parallel among independent data sets) coupled with advancing the exploration in parameter space even with partial gradient or Hessian information, if line-search or trust-region criteria are met (Petra and Anitescu 2010).

VIII.3.2.2 Scalable methods for high-resolution spatio-temporal uncertainty

Current approaches for spatio-temporal uncertainty do not scale well to the high-resolution required by CESM, in particular, atmosphere and land components (such as the one required by structural uncertainty analysis in Section VI.3) due to their reliance on direct linear algebra techniques. Furthermore, using ad hoc covariance models may lead to incompatibilities between the uncertainty description and the restrictions presented by the underlying physical processes. We recently demonstrated a matrix-free approach for Gaussian processes for carrying out both model fitting and sampling of large-scale Gaussian processes (Chen et al. 2009). Moreover, we have shown (Constantinescu et al. 2007) how one can build robust covariance functions that mimic the propagation of errors through the model in the presence of uncertain physics and that can be obtained with the aid of AD techniques. We propose to explore the use of a scalable, matrix-free Gaussian process spatio-temporal uncertainty framework with physics-based covariance functions for the next-generation CESM.

VIII.3.2.3 Stochastic parameterization

Stochastic parameterization has gained increasing attention recently as a way to improve the fidelity of the model output to observations (see recent experiments with the Hadley climate model (e.g., Slingo et al. 2010). Statistical calibration of uncertain parameters, as applied across all the testbeds in this proposal, replaces fixed (and uncertain) parameters with PDFs that are the product of the (Bayesian) calibration process. One can argue that this is just the initial step in a more comprehensive treatment of uncertain parametric process models, which should explicitly account for the uncertainty in the process models within the CESM. Such treatment can be any combination of replacing parameters with stochastic (spatio-temporal) representation and a fully stochastic treatment of the parameterization itself. Either way, such stochastic representations need to be "calibrated" (e.g., spatial-temporal correlation of stochastic error processes need to be specified) in a similar way that uncertain parameters are calibrated in current nonintrusive (Bayesian) calibration framework. We propose to investigate and explore the use of stochastic parameterization in CESM components.

VIII.3.3 Model Uncertainty

Given the active development of the CESM components throughout the CSSEF effort, which include development of new parameterization, models operating at different resolutions (including multiple resolutions), and the use of new dynamic cores, development of robust methods for model comparisons, selection, averaging, and validation are needed.

We will develop Bayesian model comparison methods employing model "plausibility." This methodology favors model parsimony and avoids over fitting. It has a built-in quantitative implementation of the Okham's razor principle, penalizing models that are too complex and that learn too much from the data (Beck and Yuen 2004). Similarly, we will use Bayesian model selection, employing model plausibility for model selection, when one model has overwhelming plausibility (Kass and Raftery 1995). We will also explore the use of Bayesian model averaging, instead of selection, for prediction of a QOI with uncertainties reflecting the marginal prediction of the set of plausible models, when there is not one model with overwhelming plausibility. This requires specifying a set of plausible models, which can be a challenge depending on the situation at hand. Further, dependences among alternate models can complicate this picture (Knutti et al. 2010). Finally, regarding model validation, we will use one subset of the data for model calibration and inference of model plausibility, while other subsets will be used for establishing agreement with model predictions, and hence validation. In this context, selection of which data to use for validation can be aided by fingerprint methods (Santer et al. 1996).

VIII.3.4 Climate Data UQ

One of the major challenges to data-driven model calibration and validation of CESM components (in particular, atmosphere and land calibration platforms), and later the fully coupled system, is the treatment of uncertainty in large, complex observational datasets, spanning multiple variables of interest. We plan to explore and develop methods in collaboration with the CSSEF Data Infrastructure and Test Bed (DIT) team to (1) estimate uncertainty in observational data products, (2) fuse information from multiple data sources, and (3) develop efficient dimensional reduction methods.

Data uncertainty estimation focuses on assigning uncertainty values to the observational data sets from the CSSEF's testbed team. The source of observational data uncertainty include (1) sensor manufacturing uncertainty, (2) missing data due to sensor failure or weather conditions, and (3) the derived data uncertainty due to different spatio-temporal averaging of observational data sets. There are a number of existing methodologies we plan to explore and expand on, including kriging-based methods (Cressie 1991) for missing data and similar statistical models for spatially and temporally misaligned/aggregated data sources.

Multiple sensors can be deployed to collect multiple data sets, which can provide better visibility and complementary information than using a single sensor. This calls for UQ techniques that aim at fusing together information from multiple sensors (Webb et al. 2001, Chong 2000, Hashemipour1988, Mori 2002) for effective use in model calibration and prediction validation. A good example of this is in the atmosphere calibration platform, which leverages multiple observations at selected ARM sites (see Section IV.2). We will develop efficient algorithms to simultaneously use the multi-sensor products in calibration of the CSSEF testbeds through competing likelihoods.

In addition to development of methods to assess uncertainty in observations and methods for sensor fusion, we will develop effective methods for dimensional reductions. In many cases, the initial/boundary conditions for CESM simulations are heterogeneous and subject to uncertainty. The stochastic input data dimensional reduction technique we propose aims to employ effective algorithms to both reduce and smooth the stochastic high-dimensional input to a stochastic low-dimensional support space and also generate (perturb) uncertain input data, as is called for in, for example, the CAM and CLM testbeds. We propose to explore the use of kernel principle component analysis (KPCA) (Scholkopf 2002, Shawe 2004, Mika 1999, Rathi 2006) for this purpose.

Both current and future CESM simulation will generate large-scale output data sets. The objective of output data dimensional reduction is to perform stochastic data reduction, reduce the output data size and extract the coherent structure and important features from the output data sets generated by high-resolution CESM simulations. Here, we propose to explore the use of a distributed "local refinement" stochastic principal component analysis (PCA) (Qu et al. 2002) approach to extract important features from the large-scale distributed data sets. We note that the PCA-based dimensional reduction approach yields a low-dimensional representation which can be leveraged to build an efficient surrogate model for multivariate output data for sensitivity and calibration.

VIII.3.5 UQ for Coupled Earth System Models

The fully coupled CESM connects the atmosphere, ocean, sea ice, land ice, and terrestrial model components to model climate. In principle, only fully coupled model calibration and prediction UQ is appropriate. However, some physical data are practically specific to certain model components since their information about model parameters is insensitive to activity in the other model components (e.g., ocean temperature profiles, ice sheet movement measurements, terrestrial vegetation CO_2 flux). For these data sources, calibration of separate component parameters will likely be quite accurate. However, model parameters that are sensitive to the coupling in the Earth system model will, in principle, require an ensemble of partially or even fully coupled climate simulations.

How one constructs these ensembles, ranging from separate to partially coupled to fully coupled model runs, including the use of reduced-order (e.g., coarser-resolution) models–and how one puts them together–can greatly impact the required computational burden for CESM UQ. This requires future research in how such coupled climate UQ can be best carried out, which we plan to initiate under this effort.

VIII.4 UQ MILESTONES AND DELIVERABLES

The milestones and deliverables for the crosscutting and long-term research in the CESM UQ are driven by the needs of UQ in the components and the long-term goal of UQ of the coupled CESM components. In particular, the advancement of core climate UQ methods are mainly driven by the initial needs of the UQ work in the three components while advancing climate UQ science is geared to both advancing current UQ methods and looking further ahead and complementing the specialized UQ tasks in the three components, which are mainly geared toward model advancements.

The UQ activities within the three components follow a similar pattern: establishing an ensemble simulation platform for the model in question; conducting initial sensitivity analysis due to uncertain parameters; preparing observations and metrics for calibration (input UQ); and then any combination of forward UQ, model validation, comparison, or selection. The process is repeated in some cases to some degree corresponding to advancements and improvements in the component models. This very much defines the milestones and deliverables for the development of core climate UQ methods, starting with adapting existing methods for sensitivity and exploratory analyses (which rely on surrogate models in most cases), followed with calibration methods, and finally introducing forward UQ and model uncertainty methods. Those methods are advanced as needed, given feedback from the component UQ.

The following provides a broad overview and timeline for proposed milestones and deliverables under the crosscutting and long-term climate UQ work.

Year 1

The first year will mainly focus on implementing and testing production-ready UQ methods in collaboration with the UQ activities in the testbeds, with the initial focus on methods related to sampling, sensitivity analysis, and surrogate models. In parallel, we will advance some of the relevant UQ methods, in particular adaptive sampling for ensemble construction and surrogate models for high-dimensional I/O data. In addition, initial work will be carried out for AD-based optimization and Bayesian methods for calibration, and on methods for climate data UQ. The major tasks are therefore as follows.

- Implement and test production-ready UQ tools in collaboration with testbeds
- Begin initial advancement of adaptive sampling methods for ensemble construction
- Begin initial advancement of surrogate models for high-dimensional input/output data
- Research an efficient, scalable Bayesian calibration framework in all testbeds

- Research AD-based optimization for calibration in the land testbed
- Identification of datasets for climate data UQ and evaluate data UQ methods

Years 2–3

In Years 2–3, we will slowly move emphasis away from sensitivity analysis to calibration, forward UQ, and model UQ (validation in particular). This still requires advancement of efficient sampling methods and surrogate models, but in particular advancement of scalable and efficient (Bayesian) calibration methods that can utilize multiple, heterogeneous data sets, including methods for dimensional reduction and the treatment of structural error. The main tasks are therefore as follows.

- Further advance adaptive sampling methods and surrogate models for calibration
- Develop and apply efficient and scalable Bayesian calibration methods across all components, including methods to leverage multiple datasets and to account for structural error
- Characterize uncertainty in observations using climate data UQ methods; use in calibration
- Test and apply AD-based optimization for calibration in land testbed
- Develop forward UQ and validation methods and apply in components
- Conduct initial exploration of efficient methods for UQ of coupled systems

Years 4–5

In Years 4–5, we will further advance the full CESM UQ framework, including the areas of sampling, sensitivity analysis, model calibration, and model UQ (particularly validation), and to apply the advancements to improved model components. There will be added emphasis on methods for model UQ, particularly model validation and selection, given new improvements to component models. The main tasks are therefore as follows.

- Further advance and refine the full UQ framework initiated in Years 1–3, particularly regarding efficiency, scalability, and robustness, given feedback from application in components
- Develop and advance model UQ methods to evaluate improvements in components
- Research and test efficient methods for UQ on coupled systems
- Outline the path forward to UQ of the fully coupled CESM

IX. TESTBED AND DATA INFRASTRUCTURE

IX.1 INTRODUCTION

The testbed and data infrastructure (TDI) component of the CSSEF project will enable the development of a new climate modeling methodology that reduces uncertainty through the provision of (1) a testbed for the rapid development and assessment of new model components (2) relevant data products, and (3) data and computing infrastructure.

This work will be driven by requirements from both model components (atmosphere, land, and ocean) and the overall global climate model. In addition, it will use existing technologies, standards, and expertise to build a unique turnkey operation suitable for CSSEF planned studies, designed experiments, testbeds, and large-scale data distribution. In so doing, we will provide a powerful platform for uncertainty quantification (UQ) in climate models and for rigorous, replicable, and transparent testing of climate science theories for a sustainable energy future.

IX.2 SCIENCE GOALS FOR THE TESTBED AND DATA INFRASTRUCTURE

IX.2.1 Testbed

To achieve the CSSEF science goals, the project will develop a new climate-model testbed infrastructure comprising two major capabilities: a calibration platform where UQ techniques are used to calibrate a model against regional observational data sets, and a validation platform where simulation quality is quantified against global observational data sets. It will be necessary to be able to adapt the testbed infrastructure to the specific requirements of each of the science areas, integrate closely with the modeling activities and UQ methods, and provide access to the (derived) data products created to meet the needs of the testbed. To avoid these activities becoming a source of delay and error, we need to automate many of the associated processes.

Workflow and provenance technologies are needed to support testbed and UQ activities, such as ensemble analysis, observational data intercomparison with model data output, initial and boundary condition UQ, and quantification of observational data set uncertainty (Walker 2009). To enable reproducibility, testbed activities must be captured in a representative workflow, thereby allowing automation of subsequent experiments, reproduction of an experiment, and validation of results (Tyer 2007). These provenance data must include both the workflow used to generate a derived data product and details on the origins of any input data. Mechanisms to capture the source or origin of a data set, subsequent transformations, and passage of the data through its various owners over time serve to document an experiment. To avoid these activities becoming a bottleneck and potential source of error, TDI will develop a framework for automation of these activities.

Without a clear paradigm shift in how large-scale data sets are handled and analyzed, the avalanche of data will overwhelm current data analysis tools and data models. These requirements push the boundaries of data analysis as data sets from high-resolution models may exceed tens or even hundreds of terabytes. Local high-resolution modeling activities conducted in some testbeds will use ensemble analyses to generate many (tens to thousands) of smaller (~1 TB) data sets, requiring data-analysis tools that are fully parallelized for large-scale data-intensive computational environments. Needed analytical tools will include multivariate statistical analysis, standardized model evaluation metrics that can operate across multiple grid resolutions, regridding tools for ocean and atmosphere, and other data assimilation and summarization tools. To support automation of ensemble analysis, robust data-model and analysis tools for climate model data sets must be developed.

IX.2.2 Data Products

Effective support of the testbed and UQ activities will require the creation of, and/or access to, relevant observational data to produce multivariant data products, infrastructure support for model development, UQ, and testbed activities.

CSSEF science will require data sets from many sources, such as:

- *Atmosphere.* climate modeling best estimates, scanning precipitation radars [e.g., Atmosphere Research Measurement (ARM) Climate Research Facility (ACRF) cloud radars and instruments (see Table IV.2)]. Further data sources will be required for the validation platform (e.g., IBTrACs, Global Precipitation Climatology Project (GPCP), Calipso, CloudSat, European Centre for Medium-Range Weather Forecasts (ECMWF), Climate Variability and Predictability (CLIVAR) Madden Julian Oscillation (MJO) (see Table IV.3)].
- *Land.* C-Lamp, AmeriFlux, FluxNet, the Moderate Resolution Imaging Spectroradiometer (MODIS) from the ORNL Distributed Active Archive Center (DAAC), U.S. Forest Service (USFS), Landsat, the National Oceanic and Atmospheric Administration (NOAA) Earth System Research Laboratory (ESRL) Global Monitoring Division (GMD), and the National Science Foundation (NSF) Long-Term Ecological Research (LTER).
- *Ocean.* the Hadley Centre, the National Snow and Ice Data Center, the Global Ocean Data Analysis Project, International Comprehensive Ocean-Atmosphere Data set, World Ocean Database, World Ocean Atlas Series.

CSSEF scientists require an infrastructure that provides search capabilities for, storage of, and access to these observational data as well as simulation data generated by CSSEF research. This infrastructure must address six major issues: data standards, data collection, data annotation, data storage, data dissemination, and data analysis. It must support a wide range of data types, support CSSEF-specific workflows, and in general provide a secure data repository for the CSSEF community.

For data discovery and access, the project will need to address the mapping of metadata vocabularies, security, and access mechanisms to both metadata and data products within other networks and data sources (Woolf 2009). In particular, such mapping will be necessary for areas that are not naturally covered by the Climate and Forecast (CF) standard. In addition, vocabulary and mechanisms to identify and access regimes or features within the data need to be aligned (Stock 2007).

Meeting the science goals of CSSEF also requires access to a wide range of data processing and analysis methods, including methods for generating derived data products with associated uncertainty information.

IX.2.3 Infrastructure

CSSEF testbed work (in particular UQ) will require access to both large-scale simulation environments and platforms optimized for data-intensive workloads (Bell 2009). We assume that CSSEF will have access to substantial computer-time allocations at DOE leadership computing facilities (LCFs) at ANL (ALCF) and ORNL (OLCF), as well as to other systems, and thus will have no need for dedicated computational resources.

CSSEF data storage requirements will also be substantial. Testbed simulations will require parallel input/output (I/O) environments (Oral 2010) that provide a structured data model suitable for parallelization and automation of ensemble analysis and intercomparison of models and observational data sets. Observational data set sources are distributed worldwide and use a variety of data formats and metadata models (Pouchard 2003, Madin 2007, Devarakonda 2010). We will establish dedicated storage systems at ALCF and OLCF. Efficiently moving data sets to and from remote locations will require integrating and tuning bulk data movement tools within the infrastructure. The ability to move data at high speeds among CSSEF sites is critical to CSSEF goals. *High speed* here means end-to-end (disk-to-disk) data movement at close to peak network speed over 10 Gbps or 100 Gbps networks. A federated data model is required to allow data sets to be generated and archived at each facility while providing transparent access to all data sets from any location (Williams 2009).

IX.3 TESTBED AND DATA INFRASTRUCTURE ARCHITECTURE

CSSEF success will depend in part on the ability of the TDI component to provide an infrastructure that can satisfy the science-driven technical requirements of the project, and do so rapidly, leveraging existing services and developments. A key building block for the CSSEF infrastructure will be the Earth Systems Grid (ESG) (led by Dean N. Williams). By building and expanding on the existing ESG, the project will ensure that the access, storage, movement, and analysis of the large quantities of data to be processed and produced by CSSEF can be performed smoothly and efficiently. To create this new environment and achieve CSSEF goals, the project team proposes to

- Advance the development of existing ESG tools in support of CSSEF's science mission, primarily by delivering the required observational data sets at resolutions and formats required by atmospheric, land, and ocean testbeds and supporting sharing and preliminary analysis of simulation output among the CSSEF team
- Provide, in a single environment, tools for converting observational data to multivariate and process-oriented data sets for model testing and methods for estimating uncertainties in the data to the extent feasible for model evaluation and parameter estimation
- Create a single framework under which the science goals for atmosphere, land, and ocean components and UQ and testing in each can be accomplished
- Allow the workflow of model testing and uncertainty quantification to be captured in a workflow and provenance environment
- Create a rapid development coupled model testbed with integrated access to customizable observational and derived data products for model verifications and UQ

In addition to ESG, the project team will work closely with the ARM program (Program lead, Jim Mathers, PNNL), visualization and analysis projects funded by BER, such as Parallel Analysis Tools and New Visualization Techniques for Ultra-Large Climate Data Sets project (PI, Robert Jacob, ANL); Ultra-scale Visualization Climate Data Analysis Tools (UV-CDAT) project (PI, Dean N. Williams, Lawrence LLNL); and Visual Data Exploration and Analysis of Ultra-large Climate Data project (PI, E. Wes Bethel, LBNL).

IX.3.1 Integrated Conceptual View

Testbed activities for each component share a common theme and process as captured in the integrated conceptual view illustrated in Figure. IX.1. Central to all activities is a workflow incorporating ensemble analysis of model simulations coupled with quantification of input and model uncertainty.

As an example, consider the testbed assessment of a new process model within a model component. The testbed will first conduct a baseline assessment of the current component, using ensemble simulations to quantify the component's input parameter sensitivity in order to reduce the dimensionality of the calibration. Illustrated in Figure IX.1 is the baseline ensemble loop in which model simulations are conducted using a variety of input parameters generated by the UQ Ensemble Driver. The UQ Ensemble Driver will analyze these ensembles and determine new input parameters for further evaluation of the baseline model's input sensitivity.

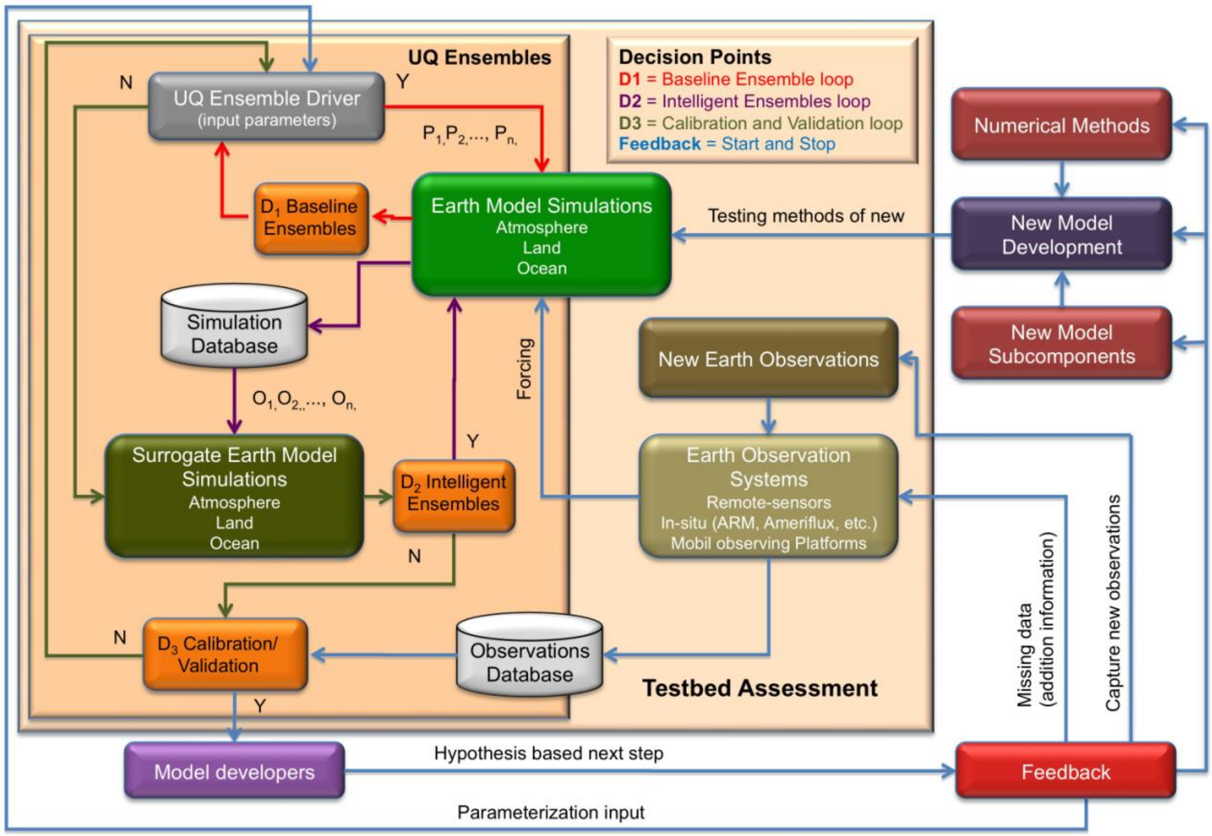

Figure IX.1. An integrated conceptual view of the baseline ensemble loop in which model simulations are conducted using a variety of input parameters generated by the UQ Ensemble Driver. This loop works for atmosphere, land, and ocean, though there are other iterative loops for model development not shown in the figure.

The second step in the UQ process is illustrated by the Intelligent Ensembles loop illustrated in Figure IX.1. For a given set of ensembles generated by the component model simulations, a set of surrogate component model simulations will be run. These surrogate simulations will be used to assess the uncertainty inherent in the parameters and process model and will generate a select set of ensembles of interest that will be re-evaluated using the baseline model for intercomparison.

The third step is the Calibration and Validation loop illustrated in Figure IX.1. This process evaluates the intelligent ensembles and confronts these model results with observational data sets to further calibrate and validate the model. Calibration will result in further input to the UQ Ensemble Driver and further analysis of both model and input uncertainty. Validation will be provided to inform model developers as to both the uncertainty of simulation results and the resultant model performance.

While each testbed will focus on specific areas of model development, such as cloud formation in the atmosphere model and mixing parameterization in the ocean model, this workflow will remain largely consistent across the testbeds. This commonality will allow testbeds to leverage common architecture elements.

The large volume of data and the geographic distribution of testbed and UQ activities will require an end-to-end architecture that supports federated data management and remote data access and management of multiple hierarchies of storage from tape archives, to disk cache, to solid-state drives. Our product architecture will provide direct support for provenance, workflow, data management, and data analysis by leveraging synergistic activities. These technologies will be tailored to the specific needs of CSSEF while developing entirely new technologies to support advanced ensemble analysis and intercomparison.

TDI must provide access to both raw data and CSSEF-derived data products, covering un-calibrated data (usually in a custom format) and potentially containing noise and artifacts (e.g., National Aeronautics and Space Administration [NASA] Level-1 products) and data that have been quality-controlled and extensively validated (e.g., NASA Level-2 products). We will develop derived data products, which have undergone uncertainty assessment using appropriate statistical and UQ tools.

There are three difficulties in using point-wise data to evaluate climate models: (1) the discrepancy in temporal and spatial scales between point observations and model output, (2) missing data, and (3) deriving geophysical parameters from remotely sensed data. Therefore, point observations need to be averaged in time and height or be converted to probability distribution functions (PDFs) or joint PDFs in order to be compatible with, and comparable to, model output. Many geophysically important quantities (such as ice water content) cannot be measured directly by remote-sensing instruments but must be derived from measurements of other observables. In addition, combining disparate data, such as remotely sensed and in situ observables, will require additional tools for regridding, assimilation, conversion, and UQ.

Challenges for atmospheric data sets stem from the wide variety of data sources that need to be integrated; ocean data suffer from their relative paucity, and land data are highly heterogeneous and generally not integrated. Generating appropriate data sets for model calibration and validation is therefore highly resource intensive. To enable rapid model development, we will automate generation of derived data products, permitting researchers to share and reuse common processing steps, as well as complete pipelines (see Figure IX.2).

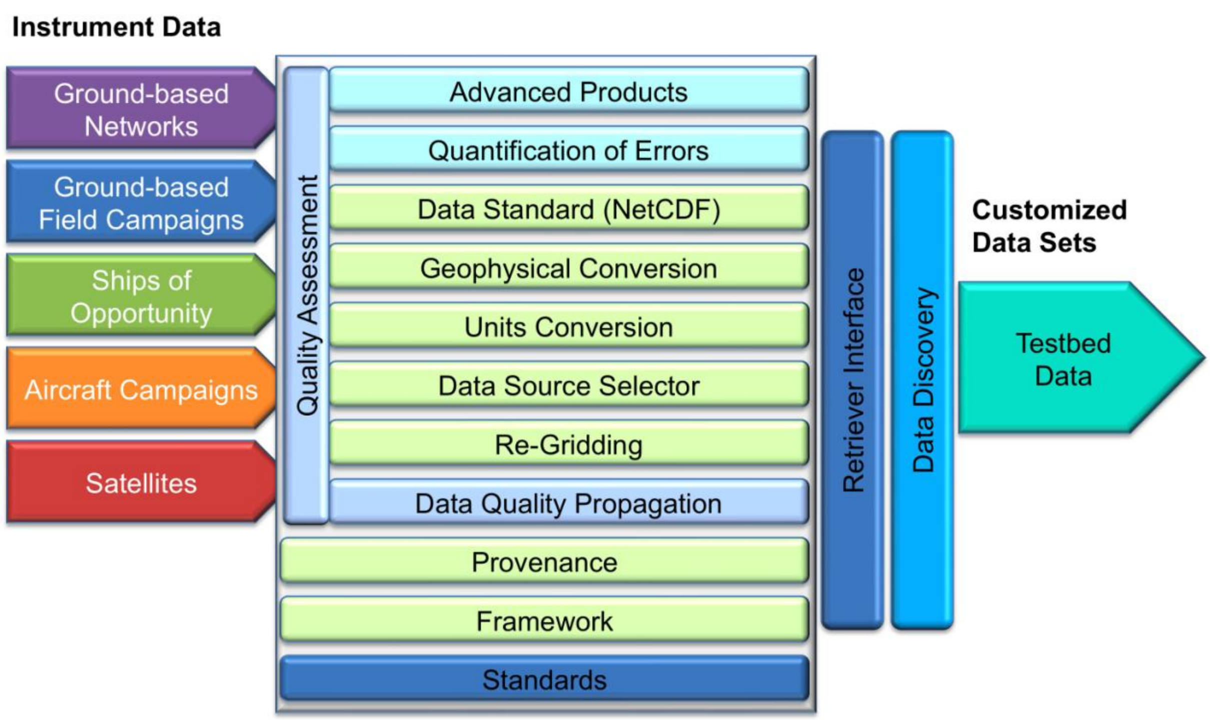

Figure IX.1. Data are collected from a wide variety of sensors, external instruments, and campaign instruments. Data quality assessments are preformed to ensure the quality of the data collected by these sources. Data retrieval and discovery mechanisms are used by the CSSEF testbed for model verifications and uncertainty quantification.

IX.4 RESEARCH AND DEVELOPMENT PLAN

We envision the software product developed under CSSEF to provide a single point of access to methods for discovering observational data sets suitable for climate evaluation, methods for converting additional data sets to climate-ready products, an environment to configure and analyze large ensemble simulations required for UQ and parameter estimation, algorithms to diagnose model results and find and characterize feature and regimes within them, and visualization and analysis methods supporting UQ. Such an ambitious outcome will only be possible by building on previous work such as the Earth System Grid-Center for Enabling Technologies (ESG-CET), funded by the Scientific Discovery through Advanced Computing (SciDAC), and recently funded BER projects in climate visualization and analysis.

IX.4.1 Integrate Additional Data Sources into ESG

While the climate modeling communities have made great strides in integrating their efforts to enable easy discovery of model outputs through activities such as ESG, the Program for Climate Model Diagnosis and Intercomparison (PCMDI) Earth System Curator (http://www.earthsystemcurator.org/about/), Europe's Metadata for Climate Modeling Digital Repositories (METAFOR) (http://www.metaforclimate.eu/), or the Global Organization for Earth System Science Portals (GO-ESSP) (http://go-essp.gfdl.noaa.gov/), the links to the observational/meteorological community are far less well developed. Major obstacles in this endeavor are the means to identify suitable observational data sources worldwide, the ability to query the data with terms familiar to modelers (the vocabulary used in climate-modeling outputs and basic observational data sets to describe the same feature or regime is often quite different), and the ability to read the data if they are not in the commonly used Network Common Data Format (NetCDF).

This project will build links with observational networks and data providers and collaboratively build integrated discovery, access, and assessment capabilities. To support observational data intercomparison and enhanced derived data products, the project team will extend ESG to support multiple data formats within the infrastructure to include NetCDF Climate and Forecast (CF) Metadata Convention—Intergovernmental Panel on climate Change (IPCC) climate model data, Hierarchical Data Format Earth Observing System (HDF-EOS)—some DAAC data sets, NetCDF (no CF compliance—AmeriFlux data sets), and raster formats (U.S. Geological Survey [USGS]—Earth Resources Observation and Science). To ease model verification and derived data-product generation, the team will create automated mappings between non-CF-compliant data set variable names and CF-compliant standard names and work within the CF Standard Names Committee to adopt new standard names for observational variables when needed. To seamlessly access data archives beyond ESG, Web-services modules will be developed to allow access to disparate observational data sources using the Open Geospatial Consortium (OGC) Web-services model (Shaon 2009, Ganguly 2008). To support derived data products, a schema discovery and integration framework will be developed to integrate climate-model data with observational data sets, leveraging existing open-source capabilities in tools such as Geospatial Data Abstraction Library (GDAL) and GDAL Open-Source Geospatial Library (OGR).

Climate model/observational data intercomparison has traditionally required modeling teams to collect observational data sets from multiple (often disparate) data systems, transform observational data sets (regridding, reprojection, format conversion, and spatiotemporal aggregation), and conduct specialized data analysis (Fast 2010). The project infrastructure will provide integration of these disparate data sets into a single federated data archive (ESG-CET), automate retrieval and transformation of observational data sets to suitable formats, and provide infrastructure for model/data comparison, including diagnostics and UQ.

To enable access to observation, simulation, and derived data, we will establish three gateways to accommodate the planned atmospheric, land, and ocean testbeds needed by CSSEF. These gateways will be federated such that a user can log onto any of the three (or more) gateways to search, browse, access, and display all data within the entire enterprise system. Domain-specific data nodes will connect to their designated gateway providing access to model data input and output data sets and observational data sets for each testbed. These data nodes will be co-resident with computational resources at the ALCF and OLCF.

IX.4.2 Derived Data Products Suitable for UQ and Testbed Activities

To fully evaluate high-resolution models, diagnostics packages must be enhanced with a focus on multivariable relationships, production of higher temporal and spatial resolution (or multi-resolution) statistics, and intercomparison with derived data products that integrate diverse observational data. Tasks and challenges include (1) identifying key parameters or multivariable relationships needed to constrain or evaluate the model; (2) identifying existing data sets containing these parameters; (3) merging observations in time and space from multiple observational platforms; (4) adding uncertainty estimates to data; and (5) deriving appropriate statistics (means, PDFs, joint PDFs) in comparable ways from observations and models. Diagnostics must include methods of separating and clustering the observations and models into analogous dynamical regimes that are useful in reducing the bias from sampling errors associated with random errors introduced by variability between regimes. For detailed point observations, such as those from ARM sites or in the ocean, obstacles to creating derived data products for model evaluation include putting data sets onto a common grid, dealing with missing or bad data in ways that do not bias the statistics, and averaging the point observations to larger spatial scales. The main challenge is posed by the paucity of ocean data. The data are mainly for the ocean surface, but little exist for the bulk of the ocean below.

To speed up the development of derived multivariable data sets, we will create together with the CSSEF scientists flexible tools to perform a variety of functions, such as averaging or subsampling when regridding and dealing with missing data, quantification of uncertainties and grid sparse observational data sets. In some cases the desired geophysical quantities do not exist as standard products and will require scientific development to produce the derived products. In developing these tools we will leverage methods recently developed for the ARM Southern Great Plains (SGP) site to many of the data sets considered critical for the proposal. These methods yield a data ensemble that can be used to quantify uncertainty in interpolated data, thereby leading to better observational constraints on verification. Multiple realizations will enable uncertainty estimation in the interpolated observations, which is crucial when being used for climate model evaluation. We will also leverage the Integrated Software Development Environment (ISDE), a framework designed to encourage the sharing of tools for common functions, such as gridding and geophysical conversions. Averaging/statistical tools developed to derive needed multivariable data products for the testbeds and algorithm development for new products will be integrated within ISDE.

Many existing data sets do not include rigorous uncertainty estimates. Thus a key challenge in using derived data products for UQ and model evaluation is assigning uncertainty values to the observations. For any derived data product we will systematically quantify uncertainty of observations and provide provenance (explicitly tracking the steps taken to create the derived product from the raw data), thereby enabling reproducibility and transparency. We will explore a number of methods for including UQ in standard derived data products, such as Climate Modeling Best Estimate (CMBE) (Xie 2010), Radiatively Important Best Estimate (RIPBE) (Shippert 2010), and CloudNet (Illingworth 2007).

IX.4.3 Infrastructure to Support Large-Scale Ensemble Runs for Model Testing and UQ

Model configuration, model execution, data storage, data analysis, and other related steps associated with a climate model simulation have become increasingly time consuming activities as climate models become more complex and data volumes grow. An increased focus on uncertainty analysis in CSSEF leads to a need for large ensemble simulations, which further increase the management process overhead and complexity. To avoid these activities becoming a bottleneck and a potential source of error, we will develop an Ensemble Data Analysis Environment (EDEN) to allow the capture of climate-model simulation state at intervals defined by the modeler, input parameters to the climate-model simulation run, relations to previous climate-model simulations, and automation of ensemble-analysis tasks. EDEN will provide an integrated infrastructure for ensemble analysis through a high-performance parallel I/O interface for storing ensemble members, a parallel scripting system (Swift 2010, Walker 2009) for interactive analysis, and automated analysis functions.

IX.4.4 Domain Specific Testbed and UQ Diagnostics

The testbed framework will generally focus on (1) quantification of parametric uncertainties and optimization of model parameters and (2) quantification of structural uncertainties. This work will involve automated comparisons of observational-data variables with metrics from ensembles of model runs. Inverse models and Bayesian techniques will be used to infer or tune parameters and provide parametric uncertainties; i.e., quantify the uncertainties on those parameters (see Sect. VIII.2). Sensitivity analysis will be used to reduce the dimensionality of these calculations (see Sect. VIII.2.1), and surrogate models will be used to make this problem tractable for computationally expensive models (see Sect. VIII.2.2). Parametric-tuning (i.e., calibration) runs will be performed in modes that are sensitive to particular sub-models or processes and compared with relevant observational data sets (see Sect. VIII.3.4). The resulting PDFs will be sampled in ensemble runs of the global-component or coupled model to derive the model predictive uncertainties associated with the parametric uncertainties. Structural uncertainties will be assessed statistically from ensembles of model runs with different structural components, such as resolution or physical assumptions. For model validation, the global-component model or coupled-model predictions will be compared with relevant global observational data sets to assess model error or discrepancies.

For the atmospheric testbed, the model will be run in either the climate (observed sea surface temperature [SST] and sea ice) configuration for model validation or in the weather-integration (nudged) configuration for model calibration and in both stand-alone and coupled modes (e.g., Phillips 2004, Williamson 2007, Hannay 2009). Model validation will be based on comparison with global (e.g., satellite) data sets, and model calibration will be based on comparison with regional (e.g., ARM) data sets.

For the land-model testbed, point or single-column measurements will be used for parameter UQ, global parameter sensitivity analysis and optimization, and quantification of uncertainties associated with forcing on Community Land Model (CLM) 4 with no feedbacks. Global gridded data will be used for global parameter sensitivity analysis and optimization, structural uncertainty quantification (e.g., using different soil models), and uncertainties due to forcing on CLM4 using Community Atmosphere Model (CAM) 5 with atmospheric feedbacks (Dickinson 2006).

For the ocean-model testbed, a numerical testbed will be developed for simple test cases. High-resolution, double-gyre model runs will be used as truth for uncertainty quantification for these cases. The global model will also be compared with observational data for validation, but autotuning of parameters will not be implemented for this testbed.

IX.4.5 Feature and Regime Characterization Cataloging and Access

As the number of multivariable data sets expands to include field campaigns for other parts of the globe and for different seasons, specialized measurements, and long-term monitoring data (e.g., ACRF sites, satellite), the project team must move beyond the historical time-series data approach to a more flexible structure in which “features” or dynamical “regimes” can be easily and analogously identified in both data sets and model output (Fast 2010, Stock 2007, Millard 2007, Woolf 2006). In the past few years, analysis techniques have been developed that move beyond simple time-series comparisons to test the models’ ability to predict observed responses to changes in dynamical conditions, such as those that might be observed during climate change. For example, data and model outputs have been binned into regimes using simple dynamical (500 millibar vertical velocity) and meteorological (lower tropospheric stability) parameters or using multivariable classification with neural networks.

Steps required to enable this type of analysis using the proposed integrated multivariable data sets and model testbeds include (1) defining the types of features or dynamical regimes that will be of interest and can be defined in both the observational data sets and model output, (2) defining formal descriptions and classifications of such features and cataloguing these criteria, (3) capturing enough metadata so that large data sets can be easily sorted and the relevant profiles extracted based on the metadata or simple 1D fields, and (4) linking observational data sets to appropriate reanalysis fields for cases where all relevant dynamical fields are not available in the observational data set. The work will build on experiences at both PNNL and the UK Natural Environment Research Council (NERC) DataGrid (Latham 2009).

IX.4.6 General Tools to Support the Collaborative Work and Smooth Operations

Testbed and UQ activities will require advanced data-analysis and visualization tools. BER recently funded three visualization efforts, primarily focused on the growing visualization demands of the data-rich climate-modeling community. We will incorporate these advanced scalable visualization techniques into the data-intensive CSSEF infrastructure, augmenting and extending their functionality where required.

One example of where extensions will be required is related to multi-sensor/multi-resolution data. We will develop algorithms to analyze and visualize both multi-sensor measurement data and multiple multi-resolution simulation data. For multi-sensor data UQ visualization, we will develop a data visualization UQ interface to reconstruct the structure and quantify the associated uncertainty by fusing multi-sensor data sets and visualize the averaged value and error bar of the multi-sensor data. For multi-resolution simulation data UQ visualization, we will develop a data UQ visualization tool to obtain the statistics from the multi-resolution ensemble simulation data sets and visualize the averaged value, the error bar—the confidence interval and risk assessment for decision-making. To quantify the uncertainty associated with the effect of resolution, we will characterize, determine, and visualize the resolution-related uncertainty on the multi-resolution simulation data sets by comparing different resolution results over testbed domains in collaboration with testbed developers.

A second area in which extensions are required relates to parallelization. Existing data analysis and visualization tools such as Climate Data Analysis Tools (CDAT) are single-threaded applications that must be modified to accommodate the more powerful ensemble analysis needed for the CSSEF initiative. We will work with the BER-funded visualization teams to scale the chosen analysis tool(s) to perform highly complex functional analyses. This process will require a multi-step process for coordinating analysis pipeline work. This process will have to be managed using automated workflow capabilities to control distributed processing within the infrastructure.

CSSEF represents a significant increase in the climate-component aggregation of simulation and observational data, thus demanding major advances in analysis methods. This research is inherently tied to the scientist's ability to effectively browse, search, and analyze data in a consistent infrastructure. Confronted with a huge diversity of data, scientists face challenges analyzing remote data and determining the right analysis tool to appropriately dissect the data for processing and study. Because no one tool can handle every data situation, the infrastructure must be designed to integrate tools from many sources. These tools will range from regridding methods (such as the Spherical Coordinate Remapping and Interpolation Package [SCRIP]) to dedicated analysis tools (such as CDAT). Analysis will be integrated within the infrastructure to support application/module sharing for computation, analysis, and management of large-scale distributed data. In doing so, the scientist's scope of understanding related to testbed results will be broadened.

IX.5 TESTBED AND DATA INFRASTRUCTURE MILESTONES AND DELIVERABLES

Work in Year 1 will focus on designing and building a first prototype of the CSSEF testbed, focusing on use cases that involve existing scientific climate data archives (e.g., the Carbon Dioxide Information Analysis Center [CDIAC], ARM and NASA observations). This work will include developing the libraries and techniques needed for data coordination, analysis, and visualization.

In Years 2 and 3, we will evaluate, debug, and refine the data archive and CSSEF testbed. We will also evaluate future computing capabilities, such as cloud computing and 100 Gbps networking. This work will also entail continued progress on ingesting data and developing metrics, managing data, and developing data analysis and visualization tools.

More specifically, in Year 2, we will proceed to initial development and development of the various components needed to manage and move data over the infrastructure. This work will include developing the libraries and techniques needed for data coordination. Year 3 work will focus on evaluating and debugging the overall system in real use cases with applications and listening to user feedback.

The goals for the final two years of the project will be challenging. The intermediate and final products, however, will depend critically on user feedback. The ultimate deliverable is a testbed that will facilitate rapid development of the coupled model.

Year 1

Architectural design of CSSEF testbed

- Architectural design of EDEN
- First experiments with the testbed: application to atmosphere model
- Manage and ingest sensitivity analysis for land model
- Define test problems for ocean model
- Implement first-cut diagnostics for ocean model
- Ingest data and metrics for each component
- Establish ESG data node at ANL
- Data analysis and visualization

Years 2 and 3

CSSEF testbed in use with atmospheric and land point models (integrate all components, conduct client testing)

- EDEN in use with land and atmospheric models
- Initial automation of testbed
- Ingestion of data and metrics for each component
- Automation of derived data product generation from selected sources
- Implementation of methods for structural uncertainties for atmospheric model
- Implementation of diagnostics for ocean model
- Interpolation of ocean/atmosphere model output and observational data to same spatial scale

- Data management
- Data analysis and visualization

Years 4 and 5

Ingest data and metrics for each component (all data available)

- Develop coupled model testbed capability
- Implement complex diagnostics for all components
- Manage data
- Complete at a analysis and visualization tools
- Fully automate testbed
- Fully deploy EDEN

X. LONG-TERM MEASURE

The Office of Biological and Environmental Research's climate science activity has established the following Long-Term Measure (LTM) for its programs: *Deliver improved scientific data and models about the potential response of the Earth's climate and terrestrial biosphere to increased greenhouse gas levels for policy makers to determine safe levels of greenhouse gases in the atmosphere*.

The Climate Science for a Sustainable Energy Future (CSSEF) Project is directly relevant to the LTM because it result in more accurate climate and Earth system model simulations using the internationally recognized, state-of-the-science Community Earth System Model (CESM). With its focus on the longer-term development objectives, the CSSEF will assure that the CESM will stay at the scientific forefront in climate simulation and prediction. The CSSEF investment will be leveraged through synergies with other CESM projects supported at laboratories and academic institutions.

XI. RELATIONSHIP TO OTHER PROJECTS

As was mentioned earlier, the Climate Science for a Sustainable Energy Future (CSSEF) project will be part of the larger CESM development and application enterprise. Through the following projects, DOE is a primary partner in supporting the CESM. The CSSEF will not duplicate efforts in these projects; rather, it will complement and provide an integrating structure for research performed by them. All of the projects have principal investigators who are leading aspects of the CSSEF, which may raise concerns that they will be over-committed. All are experienced project leaders who are able to balance multiple priorities. Further, the management of CSSEF will be results oriented, which provides a large measure of project discipline.

CESM Component Development

Title: Climate, Ocean and Sea Ice Modeling (COSIM)

Sponsor: DOE SC/BER

Principal Investigator: P. Jones (LANL)

Title: Improving the Characterization of Clouds, Aerosols and the Cryosphere in Climate Models

Sponsor: DOE SC/BER

Principal Investigator(s): P. Jones (LANL), P. Rasch (PNNL), S. Klein (LLNL), W. Collins (LBNL)

Title: Improving the Representations of Human-Earth System Interactions

Sponsor: DOE SC/BER

Principal Investigator: P.Thornton (ORNL) and A. Janetos (PNNL)

Title: Ultra High Resolution Global Climate Simulation to Explore and Quantify Predictive Skill for Climate Means, Variability and Extremes

Sponsor: DOE SC/BER

Principal Investigator(s): J. Hack (ORNL), P. Jones (LANL), K. Sperber (LLNL), W. Collins (LBNL)

Title: ORNL Climate Change Forcing Science Focus Area

Sponsor: DOE SC/BER

Principal Investigator: P.Thornton (ORNL)

Title: ORNL Climate Change Response Science Focus Area

Sponsor: DOE SC/BER

Principal Investigator: P. Hanson (ORNL)

Climate Data Testbeds and Data Management

Title: Climate Model Diagnosis and Evaluation, LLNL Scientific Focus Area (Cloud-Associated Parameterizations Testbed portion)

Sponsor: DOE SC/BER

Principal Investigator: S.Klein (LLNL)

Title: Ultra-scale Visualization Climate Data Analysis Tools

Sponsor: DOE SC/BER

Principal Investigator: D. Williams (LLNL), D. Bader (ORNL), P. Jones (LANL)

Title: Visual Data Exploration and Analysis of Ultra-large Climate Data

Sponsor: DOE SC/BER

Principal Investigator: W. Bethel (LBNL), D. Williams (LLNL)

Title: Earth System Grid Center for Enabling Technologies (ESG-CET)

Sponsor: DOE SC/ASCR (SciDAC)

Principal Investigator: D. Williams (LLNL), D. Middleton (NCAR)

Title: Identifying Robust Cloud Feedbacks in Observations and Models

Sponsor: DOE SC/BER

Principal Investigator: S.Klein (LLNL)

Numerical Methods and Computational Science

Title: A Scalable and Extensible Earth System Model for Climate Change Science

Sponsor: DOE SC/BER (BER SciDAC)

Principal Investigator(s): D. Bader (ORNL), P. Jones (LANL)

Uncertainty Quantification

Title: Quantification and Reduction of Critical Uncertainties Associated with Carbon Cycle-Climate System Feedbacks

Sponsor: DOE SC/BER

Principal Investigator: P.Thornton (ORNL), W. Riley (LBNL)

Title: Identifying Robust Cloud Feedbacks in Observations and Models

Sponsor: DOE SC/BER

Principal Investigator: S. Klein (LLNL)

XII. CSSEF MANAGEMENT PLAN

The management plan for the Climate Science for a Sustainable Energy Future Climate Science for a Sustainable Energy Future (CSSEF) project is based on the successful management strategy employed by the ORNL-based Bio-Energy Science Project (BESC), one of the three BER-supported Bioenergy Research Projects. Like BESC, CSSEF requires a clear organizational structure, a robust project management system, and effective mechanisms for integration across research areas and institutions. Because aspects of the CSSEF are high risk, the CSSEF must identify unproductive tasks rapidly and shift resources to the most promising research areas.

Our organizational approach and staffing plan have been developed specifically to meet these demanding and intertwined challenges. The major elements of our management plan, discussed in detail in the following pages, are as follows:

- Assemble a team of institutions and investigators with extensive experience in the development of state-of-the-science climate and Earth system models and the underlying methodologies to be deployed for model development in CSSEF.
- Employ an organizational structure that maintains the integration among the model component development and the crosscutting research themes.
- Implement proven project management, performance monitoring, reporting, and risk management systems at the CSSEF level, thereby providing the tools and structure necessary to effectively manage a complex multi-institution, multi-investigator program.
- Fill all CSSEF leadership positions with the best available individuals who offer the specific scientific and management experience and qualifications necessary to perform with distinction, regardless of institutional affiliation.
- Implement robust advisory and governance to engage the best available external scientific advice; ensure access to the full breadth of capabilities and expertise at all partner institutions; and provide efficient mechanisms for rapid problem resolution.
- We describe in the remainder of this plan how we will manage this research enterprise to minimize the risk for DOE and accomplish the goals described in the deliverables attachment.

XII.1 ORGANIZATIONAL STRUCTURE

The proposed CSSEF organizational structure, depicted in Figure XII.1, is explicitly designed to enable the CSSEF mission.

Major features of our structure and their associated benefits are as follows:

- A Project Director with full authority and accountability for all aspects of project operations, three model component development leaders, and three crosscutting research theme leaders to ensure tight integration among all project activities.
- Well-informed and timely decision-making.
- Independent oversight and review via an external Science Advisory Board (SAB) and a Board of Directors (BOD), designed to provide the best possible scientific and program management advice and to approve annual performance goals, projects and budget plans in an objective and transparent manner.

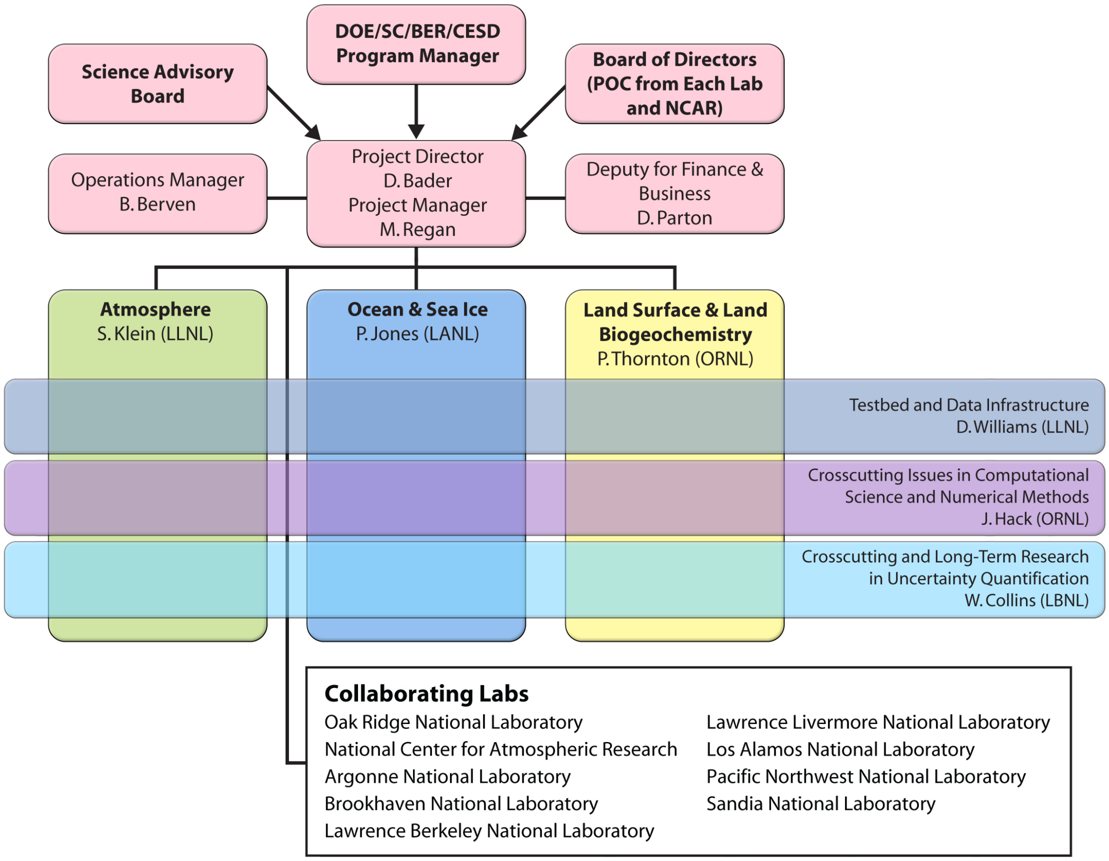

Figure XII.1. The proposed CSSEF organization provides clear lines of authority and effective vertical and horizontal integration of project activities.

- Integrated project management across multiple institutions with designated project-level practices and leads for operations and for finance and business, providing clear leadership, quality, and effective business management.
- Proven practices and tools for performance monitoring of research schedule and budget.

Key roles, responsibilities and authorities (R2A2) assigned to the CSSEF leadership roles are listed in Table XII.1.

XII.2. INTEGRATED MANAGEMENT SYSTEMS FOR PERFORMANCE

Our approach will draw on the ORNL experience in executing large technical programs that require integration of multiple technical disciplines across several institutional partners.

The Project Director (PD) will have full authority over managing the CSSEF budget, the research and development program, and project operations, upon approval of project plans and budgets by the BOD and DOE. Science leaders formally report to the PD.

CSSEF goals will be achieved through tasks carried out by staff of all the project partners reporting to science leaders within a component development effort and crosscutting theme area. Task leaders are highly accomplished researchers and have full responsibility and authority to execute the approved task plan on schedule and within budget. The Operations Manager and the Deputy Director for Finance and

Table XII.1. Each key position has clear responsibilities and authorities

Role	Responsibilities	Authorities
Board of Directors (BOD)	Review CSSEF project strategic directions	• Approve CSSEF strategic directions • Approve annual project and investment plan and performance goals for the Project leadership team • Evaluate performance of the team
Science Advisory Board (SAB)	• Advise on the scientific thrusts of the CSSEF project • Review project plans • Monitor progress toward project goals	• Assess performance of the project R&D team • Assess scientific quality
Project Director (PD)	• Provide overall leadership for the CSSEF • Single contact point for DOE CSSEF integration, capability development, integration of project activities with the CESM project	Exercise full authority to manage all aspects of the project with DOE and BOD approval
Deputy Director for Finance and Business Management	• Provide financial management and reporting • Subcontract management	• Ensure subcontractor performance • Implement effort adjustments and budget allocations so as to meet financial performance targets
Operations Manager	Managequality assurance/quality control	Approve research quality plans and monitor execution
Science Leaders	• Integrate activities vertically and horizontally across the project elements • Collectively advise the Project Director	• Develop yearly plan and budgets • Monitor progress • Implement adjustments to project plans as appropriate and approved by PD
Project Manager	• Gather project data • Generate regular reports • Monitor deliverables	Make requests and report to Director

Business Management will work with single points of contact (POCs) at all the institutions participating in CSSEF research (identified in their institution's Letter of Commitment for the CSSEF proposal). These groups will form the Operations Support Team and the Finance Support Team for CSSEF, respectively. They are fully integrated in the research enterprise and are accountable to the PD for effective support so that the science and technology team can focus on critical scientific outcomes from the CSSEF investment.

To ensure clear communication, the Science Leaders will meet with the Director, Operations Manager, and Deputy for Finance biweekly via Internet teleconference. These individuals will form the CSSEF leadership team (LT). The frequency of the meetings will be adjusted as needed to effectively manage the project progress. The PD with the project manager will prepare quarterly reports for the boards and for DOE.

The BOD serves (1) to approve the project strategic directions and annual project and budget plans, and (2) to approve annual performance goals for the project LT and to evaluate the performance of the team. It consists of representatives of the executive leadership at CSSEF institutional partners. The BOD will meet in person three times a year (or as needed). DOE will have an ex officio representative. BOD members will serve for 5 years and will elect a chair for a 2-year term. The BOD will make decisions by simple majority vote.

The SAB serves (1) to advise on the research tasks and priorities of CSSEF, (2) to review project plans, and (3) to assess scientific quality and monitor progress by CSSEF toward short-, mid-, and long-term goals. The SAB consists of up to eight internationally known scientists with extraordinary records of achievement in at least one of the areas of active research in CSSEF. DOE will have an ex officio representative. SAB members serve for 5 years, and the members will elect a chair for a 2-year term. The SAB meets annually, or as needed. Appointments to the SAB will be made after the CSSEF proposal completes merit peer-review, so as to not reduce the field of potential reviews that would result from conflicts of interest.

Performance Monitoring—The overall performance goal is to conduct comprehensive, high-impact integrated research. ORNL has proven management systems to establish the necessary contractual agreements; track accountability; and monitor budget, level of effort, timeline, and deliverable status of all work conducted by CSSEF institutions on a task basis. The role of the POCs for the other research partners is to ensure their institutions' commitment to supporting the success of the CSSEF.

The proposed scope has been organized into a Work Breakdown Structure (WBS) for identifying, defining and managing project activities. During project execution, the WBS will be expanded, as required, to lower levels (i.e., subtasks at individual institutions) to allow the necessary tracking of costs and schedule.

Performance-Based Reporting System**—**Progress will be tracked against established performance milestones and planned budgets by the ORNL business management system with data provided by the participating institutions. ORNL will provide quarterly "dashboard" type reports to DOE. These reports typically will include standard financial indicators, human resources status, technical progress highlights, and updates associated with accomplishing project milestones. They will serve the Project LT in making timely decisions concerning the execution of the project plan. The SAB will review the progress of the CSSEF research program periodically during the year.

The DOE-Oak Ridge Operations Office of the Assistant Manager for Science and the management and operating contractor (UT-Battelle) have implemented a certifiable Earned Value Management System (EVMS) that is in compliance with ANSI/EIA-748-A-1998. CSSEF will use a type of EVMS to monitor and evaluate project progress and performance for the Project's duration. Periodically, the Project performance in terms of cost/schedule/risk performance indices (CPI/SPI/RPI) will be reviewed, using an analysis of schedule and cost data to evaluate the current status and to forecast the total estimated project cost and completion. The PD will be responsible for measurement and evaluation of the progress against the goals and milestones, budgets, and schedule and for giving advance warning of trends, deviations, and other problems to facilitate timely corrective actions that minimize any impacts on cost, schedule, and quality. The Project will have a critical path resource loaded schedule (based on the WBS), which will be reviewed periodically by the Project LT.

Risk Assessment**—**We performed a preliminary risk assessment during the proposal writing process. The predominant consequence of the identified risks is a potential for cost or schedule increases in the research plan. Based on this analysis, the following activities and mitigation strategies are incorporated in the project plan:

- Continue to monitor, rank, and coordinate potential risks throughout the project. This may include considering lessons learned and benchmarking of similar projects.
- Test multiple strategies for success in high-risk areas (e.g., application of novel uncertainty quantification techniques).
- Conduct regular reviews with the potential to redirect resources or to allocate reserves.

XIII. MILESTONES AND DELIVERABLES

We have listed a set of milestones for Year 1, Year 3 and Year 5 within each section of the proposal. Below, we have rearranged the milestones to produce a composite listed by due date, rather than research area. We fully realize that dependencies exist between the component efforts and the crosscutting research themes. Nevertheless, any comprehensive roll-up of the milestones at this stage of the project development would be futile, because it would intersect with other, potentially unknown activities that are part of the CESM enterprise. The CESM Scientific Steering Committee (SSC) will soon undertake preparation of a long-term implementation plan, which will include CSSEF efforts. The Project Director (David Bader) and one of the Science Leaders (William Collins) are both members of the SSC. The first action for the CSSEF Leadership Team upon award of the project will be to develop a comprehensive project plan that integrates CSSEF tasks with other CESM development efforts and produce a roadmap by which a more consolidated view of project progress can be measured. Overall CSSEF objectives, however, remain clear, as the project will be judged by its progress in accelerating development of CESM3, particularly in the three overarching research directions identified in Chapter II, “Approach.”

As stated in the Management Plan, the Leadership Team is prepared to abandon unproductive research paths and redirect resources and effort to those showing more promise. The motivation for setting Year 1 milestones for each of the project’s research is to make this identification early, particularly for some of the higher-risk and resource-intensive tasks. After this initial winnowing, formal task evaluation will occur over two-year intervals, with informal progress checks held every 6 months.

1. Year 1

1.1 Atmosphere

1.1.1 Data and Workflow Infrastructure

1.1.1.1 Initial design and prototype of calibration testbed, including at least one data set and metric

1.1.1.2 Initial design of data archiving

1.1.1.3 Initial design for calibration data sets and metrics and validation diagnostics

1.1.1.4 Initial design and prototype of validation platform

1.1.2 Computational Science and Numerical Methods

1.1.2.1 Deliver high- and low-resolution CAM5 configurations for testbed

1.1.2.2 Deliver CAM5 variable resolution: initial configurations with refinement to 1/8° resolution

1.1.3 Uncertainty Quantification in the Atmospheric Testbed

1.1.3.1 Initial surrogate model for prototype calibration platform

1.1.3.2 Exploratory sensitivity analysis of low-resolution CAM5

1.1.3.3 Determine CAM5 physics parameters to be perturbed and their ranges

1.1.3.4 Address parameterization issues related to variable resolution grid and increased horizontal and vertical resolution, as needed

1.2 Ocean

1.2.1 Initial performance profile for prototype MPAS ocean model and identification of performance limiter

1.2.2 Implement new kinematic closure for MPAS ocean model and begin design of multi-resolution approaches

1.2.3 Formulate initial design of new ocean-ice interfaces and develop potential approaches for new momentum and tracer coupling at the interface

1.2.4 Evaluate candidate rheologies and create plan for integrating and testing new approach in CICE

1.2.5 Implement initial preconditioner in implicit version of POP model to test approaches. Begin design of implicit sea ice software design

1.2.6 Identify the initial set of model test configurations and reference solutions for validation test bed and begin creation of unit and process level test drivers

1.2.7 Identify model quality metrics for ocean and ice for the UQ applications

1.2.8 Generate initial results from UQ application to POP LANS-alpha in a channel configuration and sea-ice parameterization in a reduced resolution configuration.

1.3 Land

1.3.1 Land-Climate Feedback

1.3.1.1 Implement two-layer treatment of litter/SOM pools and fluxes

1.3.1.2 Implement and evaluate new reactive nitrogen parameterizations

1.3.2 Land UQ

1.3.2.1 Assessment of intrusive vs nonintrusive sensitivity analysis approaches

1.3.2.2 Single-point and grid-based model sensitivity analyses

1.3.3 Land Testbed and Data

1.3.3.1 Design criteria established for sensitivity analysis functionality

1.3.3.2 Sensitivity analysis functionality demonstrated

1.3.3.3 Design criteria established for land testbed data interface

1.3.3.4 Land testbed data ingest demonstrated on C-LAMP data set

1.3.3.5 Ingest C-LAMP data sets

1.3.3.6 Ingest AmeriFlux and FluxNet data sets

1.3.3.7 Initiate gridding of GHCND data set.

1.4 Numerical Methods

1.4.1 Discretization

1.4.1.1 Implementation of a verified baseline version of FV-AMR, based on the flat parallelism model.

1.4.2 Coupler Development

1.4.2.1 Implementation of MCT Data Model using MOAB classes, with MCT test cases prototyped Increase robustness of current SCRIP Package

1.5 Uncertainty Quantification

1.5.1 Implement and test production-ready UQ tools in collaboration with testbeds.

1.5.2 Begin initial advancement of adaptive sampling methods for ensemble construction.

1.5.3 Begin initial advancement of surrogate models for high-dimensional input/output data.

1.5.4 Research an efficient, scalable Bayesian calibration framework in all testbeds.

1.5.5 Research AD-based optimization for calibration in the land testbed.

1.5.6 Identification of datasets for climate data UQ and evaluate data UQ methods.

1.6 Data

1.6.1 Architectural design of EDEN

1.6.2 First experiments with the test bed: application to atmosphere model

1.6.3 Manage and ingest sensitivity analysis for land model

1.6.4 Defining test problems for ocean model

1.6.5 Implement first-cut diagnostics for ocean model

1.6.6 Ingest data and metrics for each component

1.6.7 Establish ESG data node at ANL

1.6.8 Data analysis and visualization

2. Years 2–3

2.1 Atmosphere

2.1.1 Data and Workflow Infrastructure

2.1.1.1 Working version of testbed including automation

2.1.1.2 Robust data archiving and visualization tools for atmospheric comparisons

2.1.1.3 Implementation of calibration data sets/metrics in testbed including in-line computation of second-order diagnostics to reduce input and output need

2.1.1.4 Instrument simulator modified for ground-based data

2.1.1.5 Working version of validation platform

2.1.2 Computational Science and Numerical Methods

2.1.2.1 Deliver CAM5 high-res configuration at 1/8° running efficiently on O(100,000) cores with integration rates to support decadal simulations

2.1.2.2 Optimize configurations for the variable resolutionCAM5 with respect to refinement rate, dissipation, and time-stepping

2.1.3 Uncertainty Quantification in the Atmospheric Testbed

2.1.3.1 Define sets of parameter values with equal calibration platform metrics

2.1.3.2 Explore the sensitivity of parameter sets to the method of surrogate model fitting

2.1.3.3 Provide parameterization modifications to convection, cloud, and aerosol parameterizations as needed

2.2 Ocean

2.2.1 Fix initial Performance issues with MPAS ocean model with a goal of performance equivalence to POP in similar configurations. Identify cost-benefit of advanced schemes

2.2.2 Implement additional closure schemes for MPAS-O and evaluate results at IPCC resolutions

2.2.3 Initial implementation of CICE within MPAS framework and begin testing of ocean-ice coupling ideas

2.2.4 Initial implementation of new sea ice rheology

2.2.5 Implementation of split-explicit and semi-implicit preconditioned time integration in experimental branch of MPAS Implement capability of using EVP as a preconditioner to JFNK and Trilinos solver capability in sea ice component

2.2.6 Complete prototype hierarchy of ocean test cases for validation test bed and begin development of automation scripts

2.2.7 Complete reference UQ analysis of POP-alpha and sea ice; POP projection uncertainty ensemble available for analysis

2.2.8 Begin application of UQ methods to new MPAS closure schemes Design and begin ensemble experiments for evaluating resolution and topographic sensitivity in UQ framework

2.3 Land

2.3.1 Land-Climate Feedback

2.3.1.1 Implement 14C model

2.3.1.2 Implement new nitrogen-phosphorus model

2.3.1.3 Implement fully depth-resolved litter/SOM model

2.3.1.4 Implement reactive transport algorithms for nitrogen in multi-layer model

2.3.1.5 Evaluate two alternative age-class representations against inventory data

2.3.2 Subgrid Hydrology

2.3.2.1 Implement new watershed-based hydrology structure

2.3.2.2 Evaluate options for number and structure of elevation classes

2.3.2.3 Implement new snow depth distribution model with elevation downscaling

2.3.2.4 Implement RTM as a separate coupled model component in CESM

2.3.3 Land UQ

2.3.3.1 Optimized parameter estimates for single-point and gridded model implementations

2.3.3.2 Updated sensitivity analysis and parameter optimization using CESM forcing

2.3.4 Land Testbed and Data

2.3.4.1 Design criteria established for parameter estimation functionality

2.3.4.2 Parameter estimation functionality demonstrated with single-point simulations

2.3.4.3 Finalize gridding of GHCND data set

2.3.4.4 Ingest remote sensing data sets from MODIS and Landsat

2.3.4.5 Ingest ancillary observations from flux tower locations

2.3.4.6 Ingest ARM-Carbon data sets

2.3.4.7 Ingest USGS watershed and river flow data sets

2.3.4.8 Ingest forest inventory data sets

2.3.4.9 Ingest soil C and N data sets

2.3.4.10 Ingest high-resolution disturbance data sets

2.4 Numerical Methods

2.4.1 Discretization

2.4.1.1 Coupling of the new dynamical core to CESM. Testing and validation against HOMME multiresolution hydrostatic dynamical core at resolutions where both are expected to be valid.

2.4.1.2 Implementation of hybrid parallelism in new dynamical core, and baseline measurements of performance.

2.4.1.3 Begin investigation of physics parameterizations for multiresolution calculations, with particular emphasis on finest scales at or below 3 km mesh spacing. This work will be done in collaboration with the test bed, UQ teams.

2.4.2 Coupler Development

2.4.2.1 Complete MCT implementation based on MOAB classes and methods. New prototype CPL toolkit embodying new MOAB-MCT implementation working with “data” models MOAB-based implementation of SCRIP Improved higher-order interpolation methods

2.5 Uncertainty Quantification

2.5.1 Further advance adaptive sampling methods and surrogate models for calibration.

2.5.2 Develop and apply efficient and scalable Bayesian calibration methods across all components, including methods to leverage multiple datasets and to account for structural error.

2.5.3 Characterize uncertainty in observations using climate data UQ methods; use in calibration.

2.5.4 Test and apply AD-based optimization for calibration in land testbed.

2.5.5 Develop forward UQ and validation methods and apply in components.

2.5.6 Conduct initial exploration of efficient methods for UQ of coupled systems.

2.6 Data

2.6.1 EDEN in use with land and atmospheric models

2.6.2 Initial automation of test bed

2.6.3 Ingestion of data and metrics for each component

2.6.4 Automation of derived data product generation from selected sources

2.6.5 Implementation of methods for structural uncertainties for atmospheric model

2.6.6 Implementation of diagnostics for ocean model

2.6.7 Interpolation of ocean/atmosphere model output and observational data to same spatial scale

2.6.8 Data management

2.6.9 Data analysis and visualization

3. Years 4–5

3.1 Atmosphere

3.1.1 Data and Workflow Infrastructure

3.1.1.1 Production version of testbed

3.1.1.2 Robust automated procedures for analysis/visualization

3.1.1.3 Implementation of diagnostics and metrics from new ACRF instrumentation

3.1.1.4 Instrument simulator incorporated into model diagnostics and metrics

3.1.1.5 Expanded global diagnostics of precipitation for validation platform

3.1.2 Computational Science and Numerical Methods

3.1.2.1 Deliver a CAM5 high-resolution configuration at 1/8° running at 5 SYPD on both LCFs

3.1.2.2 Fully integrate variable-resolution configurations into CAM for improved regional climate modeling

3.1.3 Uncertainty Quantification In The Atmospheric Testbed

3.1.3.1 Explore sensitivity of parameter sets to parent model configuration and the choice of site of interest

3.1.3.2 Analyze of the relative value of calibration platform diagnostics to improvement in global climate simulation

3.1.3.3 Limited sensitivity analysis of the high-resolution model utilizing parameter sets devised from calibration platform

3.1.3.4 Address parameterization computational efficiency issues as needed

3.2 Ocean

3.2.1 Continue to optimize MPAS-O model and MPAS framework with an additional focus on new hybrid architectures to be delivered in this year

3.2.2 Develop new scale-aware parameterizations for remaining physical processes represented in MPAS O (e.g., overflows, tidal mixing, sub-mesoscale processes)

3.2.3 Evaluate embedded sea ice model in ocean and related boundary schemes in full ocean-ice coupled simulations

3.2.4 Evaluate new anisotropic ice rheology in full sea ice model

3.2.5 Develop and implement globalization methods for JFNK and development of JFNK technology focused on the advanced models and discretizations as applied to sea ice problems

3.2.6 Complete a fully automated ocean/ice validation framework

3.2.7 Demonstrate ability of UQ framework to provide parameter estimation for closure schemes

3.2.8 Use UQ framework to identify regional resolution sensitivity in MPAS ocean

3.3 Land

3.3.1 Land-Climate Feedback

3.3.1.1 Introduce dependence of SOM model on mineralogy and physical structure

3.3.1.2 Assess nitrogen-as-surrogate nutrient hypothesis in global model

3.3.1.3 Evaluate influence of age-class representation on land model UQ

3.3.1.4 Evaluate prediction uncertainty associated with forcing bias

3.3.1.5 Evaluate coupled model prediction uncertainty associated with CESM/GCAM coupling

3.3.1.6 Subgrid hydrology deliverables

3.3.1.7 Evaluate influence of subgrid hydrology structure on global water and carbon fluxes

3.3.1.8 Evaluate influence of subgrid snow on global water and energy fluxes.

3.3.1.9 Implement improved river flow rate and flood parameterizations

3.3.2 Land Testbed and Data

3.3.2.1 Design criteria for prediction error propagation functionality

3.3.2.2 Land testbed interoperability with other components for coupled model error propagation

3.3.2.3 Ingest ecosystem response experiment data sets

3.3.2.4 Ingest NEON data sets

3.3.2.5 Produce synthesis of PFT descriptions

3.3.2.6 Ingest intensive field campaign data sets

3.3.2.7 Update previously ingested data sets (as available)

3.4 Numerical Methods

3.4.1 Discretization

3.4.1.1 Complete implementation of hybrid parallelism in FV-AMR, and demonstrate that it runs at scale on at least one of the next-generation LCF systems.

3.4.1.2 Extension of FV-AMR to permit vertical refinement. This capability will enable LES simulations of stratocumulus clouds.

3.4.1.3 Continue work on new multiresolution physics models, with CSRM of tropical convective storms and tropical cyclones as the target science applications.

3.4.1.4 Delivery of a version of FV-AMR that runs at scale on the second LCF system.

3.4.2 Coupler Development

3.4.2.1 Complete MCT implementation based on MOAB classes and methods. New prototype CPL toolkit embodying new MOAB-MCT implementation working with “data” models MOAB-based implementation of SCRIP Improved higher-order interpolation methods

3.4.2.2 Complete coupling infrastructure running at scale pParallel, online computation of interpolation weights for a wide variety of model meshes Regridding of vector fields across singularities and on naïve staggered grids

3.5 Uncertainty Quantification

3.5.1 Further advance and refine the full UQ framework initiated in years 1–3, particularly regarding efficiency, scalability, and robustness, given feedback from application in components.

3.5.2 Develop and advance model UQ methods to evaluate improvements in components.

3.5.3 Research and test efficient methods for UQ on coupled systems.

3.5.4 Outline the path forward to UQ of the fully coupled CESM.

3.6 Data

3.6.1 Develop coupled model test bed capability

3.6.2 Implement complex diagnostics for all components

3.6.3 Manage data

3.6.4 Data analysis and visualization

3.6.5 Fully automate test bed

3.6.6 Fully deploy EDEN

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CURRICULUM VITAE, CURRENT AND PENDING FUNDING, AND FACILITIES AND RESOURCES

ORNL and its partners have identified a comprehensive, experienced team of nationally and internationally recognized experts for the CSSEF effort. All personnel were selected because of their formal education and training, their relevant professional experience, and the reputation and scientific insight they can bring. Each has a solid understanding of relevant issues as well as an established reputation in his or her respective field, in most cases in areas of critical importance to the goals of CSSEF.

Biographical information for proposed management and research personnel follow, grouped by institution (listed in alphabetic order) and arranged alphabetically within their institution grouping. Sections containing (1) information about current and pending funding for each participant and (2) the facilities and resources at each participating research institution follow the biographical sketches.

MANAGEMENT TEAM AND SCIENCE LEADS

Name	Role	Institution
David C. Bader	Project Director	ORNL
Barry Allen Berven	Operations Manger	ORNL
William D. Collins	Uncertainty Quantification, Science Lead	LBNL
James J. Hack	Numerical Methods and Computer Science, Science Lead	ORNL
Phillip W. Jones	Ocean and Sea Ice, Science Lead	LANL
Stephen A. Klein	Atmosphere, Science Lead	LLNL
Dennis W. Parton, Jr.	Deputy for Finance and Business	ORNL
Mary Regan	Project Manager	ORNL
Peter E. Thornton	Land Surface and Land Biogeochemistry, Science Lead	ORNL
Dean Norman Williams	Data System Evolution	LLNL

RESEARCH TEAM

ORNL
Galen M. Shipman
Ross G. Miller
Feiyi Wang

NCAR
James W. Hurrell
David M. Lawrence
Mariana Vertenstein
Gokhan Danabasoglu
Richard B. Neale

ANL
Mihai Anitescu
Emil Constantinescu
Ian T. Foster
Robert L. Jacob
J. Walter Larson

BNL
Scott Edward Giangrande
Wuyin Lin

LBNL
Jeffrey Q. Chambers
Phillip Colella
William J. Riley
Margaret S.Torn

LLNL
Gardar Johannesson

LANL
James R. Gattiker
David M. Higdon
Elizabeth C. Hunke
Dana A. Knoll
Christopher K. Newman
Todd Ringler
Wilbert Weijer

PNNL
Dilip Ganguly
Kerstin Kleese-Van Dam
Guang Lin
Sally McFarlane
Philip Rasch
Chitra Sivaraman

SNL
Bert J. Debusschere
Hope A. Michelsen
Habib N. Najm
James R. Overfelt
Jaideep Ray
Laura P. Swiler
Mark A. Taylor
Timothy G. Trucano

APPENDIXES

APPENDIX 1: GUIDANCE FOR PROPOSAL SUBMISSION: CLIMATE SCIENCE FOR A SUSTAINABLE ENERGY FUTURE PROJECT

GUIDANCE FOR PROPOSAL SUBMISSION: CLIMATE SCIENCE FOR A SUSTAINABLE ENERGY FUTURE PROJECT

SUMMARY

Oak Ridge National Laboratory has been designated as the project lead for a multi-laboratory project, Climate Science for a Sustainable Energy Future (CSSEF). The objective of this project is to significantly increase the accuracy of climate models over the next decade by reducing uncertainties in models and in the data that are the required inputs for the models. The Office of Science (SC), U.S. Department of Energy (DOE), hereby requests a peer-reviewable proposal for CSSEF.

BACKGROUND

Program Objective

In 2011, Office of Biological and Environmental Research (BER) will launch the CSSEF project, which will address a critical and relatively straightforward objective–to accelerate the incorporation of new knowledge, including process data and observations, into climate models and to develop new methods for rapid validation of improved models. A crosscutting objective of CSSEF is to develop novel approaches to exploit computing at the level of many tens of petaflops in climate models. These challenges are recognized broadly in the climate community and DOE is well equipped to address them.

Climate and Earth systems science has reached a critical convergence of national need and scientific capability with regard to climate change. As the demand for greater predictive power grows and new, petaflop-scale computing capabilities come online, what is urgently needed is an integrated, multidisciplinary project designed to bring these manifold resources together in a concerted, strategic research effort designed to take global models—both general circulation and earth models—to the level where they can be genuinely predictive at the regional level. The challenge is to foster much greater integration and enhanced communication among researchers in the modeling community.

The CSSEF activity will be planned and managed in accordance with project-management processes, building on the SC's expertise in managing large-scale multi-institutional projects to produce a world-leading, integrated capability. The activity will be managed as a large, coordinated, multi-laboratory project. The researchers will not be co-located, rather CSSEF will draw from a number of national laboratories to focus the best scientific expertise on these challenges. The goal is to systematically reduce the uncertainties in predictions of decade-to-century climate change and increase the availability and usability of climate predictions to address the critical DOE mission to provide energy security to the Nation in a sustainable way. A major challenge in creating models that are truly predictive is the implementation of methods to quantify uncertainties in climate simulations and to identify, obtain, and incorporate additional observational data.

The CSSEF activities will focus on four primary activities (1) a focused effort for converting observational data sets into specialized, multi-variable data sets for model testing and improvement; (2) development of model development testbeds in which model components and sub models can be rapidly prototyped and evaluated; (3) research to enhance numerical methods and computational science research focused on enabling climate models that use future computing architectures; and 4) research to reduce the unacceptably large range of uncertainty in current models.

DATES

Formal proposals submitted in response to this notice must be received by 4:30pm, E.D.T August 1, 2010. The proposals will then be submitted for merit review to permit timely consideration for award in Fiscal Year 2011.

Please see the ADDRESSES section below for further instructions on the method of submission for the proposal.

ADDRESSES AND SUBMISSON INSTRUCTIONS

Have your LAB administrator submit the entire LAB proposal and FWP via Searchable FWP (https://www.osti.gov/fwp). If you have questions about who your LAB administrator is or how to use Searchable FWP, please contact the Searchable FWP Support Center.

Please submit, via Federal Express, a single PDF file of the entire LAB proposal and FWP on a CD along with two hard copies to the address below. This will assist in expediting the review process.

Please send the CD and 2 hard copies via Federal Express to:

Karen Carlson-Brown
Climate and Environmental Sciences Division, SC-23.1
Office of Biological and Environmental Research
Office of Science
19901 Germantown Road
Germantown, MD 20874-1290
ATTN: CSSEF

For further information contact:

Dr. Wanda Ferrell
Program Manager
Climate Science for a Sustainable Energy Future
Climate and Environmental Sciences Division
Tel: (301) 903-3281
Email: wanda.ferrell@science.doe.gov

REVIEW PROCESS

The model for the review process will be the Bioenergy Research Centers that includes a merit review of the proposal, a DOE review of the project, and annual onsite BER programmatic and operational reviews.

SUPPLEMENTARY INFORMATION

BER’s climate science activity has established the following Long Term Measure (LTM) for its programs: Deliver improved scientific data and models about the potential response of the Earth’s climate and terrestrial biosphere to increased greenhouse gas levels for policy makers to determine safe levels of greenhouse gases in the atmosphere.

In FY 2011, the following topics shall be addressed in **Climate Science for a Sustainable Energy Future Project**:

1) A focused effort for converting observational data sets into specialized, multi-variable data sets for model testing and improvement.
2) Development of model development testbeds in which model components and sub models can be rapidly prototyped and evaluated.
3) Research to enhance numerical methods and computational science research focused on enabling climate models that use future computing architectures.
4) Research to enhance efforts in uncertainty quantification for climate model simulations and predictions.

Data Sharing Policy: Research data obtained through public funding are a public trust. As such, these data must be publicly accessible. To be in compliance with the data policy of the U.S. Global Change Research Program of full and open access to global change research data, the proposal submitted in response to this guidance must include a description of the researcher's data sharing plans if the proposed research involves the acquisition of data in the course of the research that would be of use to the climate change research and assessment communities. This includes data from extensive, long-term observations and experiments and from long-term model simulations of climate that would be costly to duplicate. The description must include plans for sharing the data that are to be acquired in the course of the proposed research, particularly how the acquired data will be preserved, documented, and quality assured, and where it will be archived for access by others. Data of potentially broad use in climate change research and assessments should be archived, when possible, in data repositories for subsequent dissemination. Examples of DOE-funded data repositories may be found at http://cdiac.ornl.gov/, http://www-pcmdi.llnl.gov/ipcc/about_ipcc.php. The repository where the researcher intends to archive the data should be notified in advance of the intention, contingent on a successful outcome of the proposal review. If data are to be archived at the researcher's home institution or in some other location, the proposal must describe how, where, and for how long the data will be documented and archived for access by others. Researchers are allowed an initial period of exclusive use of the acquired data to quality assure it and to publish papers based on the data, but they are strongly encouraged to make the data openly available as soon as possible after this period. DOE's Office of Biological and Environmental Research defines the exclusive use period to be one year after the end of the data acquisition period for the proposed performance period of the award but exceptions to extend this period may be justified for unique or extenuating circumstances.

PROGRAM FUNDING

It is anticipated that up to $16,000,000 will be available for an award in Fiscal Year 2011, contingent on the availability of appropriated funds. Proposal may request project support up to five years. Out-year support is contingent on the availability of funds and on the progress of research and programmatic needs. Multi-lab research is required. Funding for this research will come from the Climate and Earth System Modeling program. DOE is under no obligation to pay for any costs associated with preparation or submission of proposals. DOE reserves the right to fund, in whole or in part, any, all, or none of the submitted proposal.

Contingent on satisfactory peer review, the approximate funding level of specific areas is indicated below:

a) Converting observational data sets into specialized, multi-variable data sets for model testing and improvement ($3M)

b) Development of model development testbeds in which model components and sub models can be rapidly prototyped and evaluated ($3M)

c) Research to enhance numerical methods and computational science research focused on enabling climate models that use future computing architectures ($4M)

d) Research to enhance efforts in uncertainty quantification for climate model simulations and predictions. ($5M)

e) Project Management ($1M)

SUBMISSION INFORMATION FOR FORMAL PROPOSAL

The instructions and format described below must be followed.

The proposal must include a one-page abstract of the proposed research. All collaborators should be listed with the abstract. Attachments should include curriculum vitae, a listing of all current and pending federal support and letters of intent when collaborations are part of the proposed research. Curriculum vitae should be limited to no more than two pages per individual. The proposal must explicitly state how the proposed project will support accomplishment of the BER climate science activity LTM.

The following is a list of essential items that a proposal must contain:

1) **Field Work Proposal (FWP) Format—**Complete and signed by appropriate officials
2) **Proposal Cover Page**
3) **Table of Contents**
4) **Budget Page(s) (Form DOE F 4620.1)—**Complete a separate Budget Page for the entire multi-year period for each separate participating institution.
5) **Other Project Information**
    a) **A one-page abstract (on a page by itself)**. The abstract should include: name of the laboratory; name of the principal investigator and the principal investigator's email address and phone number; name of the co-principal investigator(s) (if any) and their email address(es) and phone number(s); an abstract of the project narrative.
    b) **Project Narrative:** A detailed description of the proposed project (research plan), including the justification and objectives of the project, its relationship to the SC program and the researcher's plan for carrying it out. The format for the narrative should be 8.5×11-inch pages of single-spaced, at least standard 11-point type with 1-inch margins. (i) Introduction–Should contain enough background material, including review of the relevant literature, to demonstrate sufficient knowledge of the state of the science. (ii) Research Plan–The major part of the narrative should be devoted to a description and justification of the proposed project, including details of the method to be used. It should also include a timeline for the major activities of the proposed project, and should indicate which project personnel will be responsible for which activities. Include a plan that describes how the project results or resources will be disseminated in a timely manner and in an accessible and usable form to the broader scientific community.
    c) **Management Plan:** An overview of the organizational structure should be provided. This should include where the project resides within the Oak Ridge National Laboratory organization (e.g., is it within a department, or shared among departments?); the leadership structure and how it relates to leadership within the National Laboratory. This section also should describe a plan for internal interactions within ORNL and for inter-laboratory interactions with the other laboratory participants. Should outline how the work will be coordinated among the participating institutions, the overall chain of command, the communication plan, the leads for each area, the overall allocation of resources among the various partners, etc.A staffing and organizational structure chart should be provided. The proposal should provide a timeline of specific products that are associated with the four areas of research.
    d) **Curriculum Vitae:** Detailed information about the background and experience of the principal investigator and co-principal investigators. Biographical sketches are limited to two pages for the principal investigator, and two pages for the co-principal investigators.
    e) **Long Term Measure:** The proposal must explain how the proposed research will advance the BER climate science activity LTM detailed above.
    f) **Facilities and Resources:** Include information on the experience of the proposer's organization, its facilities, and resources that would be relevant to successful operation of the project, including access to high performance computing platforms capable of petaflop performance

g) **Statement of all current and pending support** for the principal investigator and co- principal investigators, including the time devoted to each project by the principal investigator and co-principal investigators.

The instructions and format described should be followed.

OFFICE OF SCIENCE GUIDE FOR PREPARATION OF SCIENTIFIC/ TECHNICAL PROPOSALS TO BE SUBMITTED BY NATIONAL LABORATORIES

The proposal from Oak Ridge National Laboratory submitted to the Office of Science (SC) as a result of this Program Guidance will follow the Department of Energy Field Work Proposal process with additional information requested to allow for scientific/technical merit review. The following guidelines for content and format are intended to facilitate an understanding of the requirements necessary for SC to conduct a merit review of a proposal. Please follow the guidelines carefully, as deviations could be cause for declination of a proposal without merit review.

1. Evaluation Criteria

After an initial screening for eligibility and responsiveness to this guidance, the proposal will be subjected to a formal scientific merit review (peer review). The proposal will be evaluated against the following criteria, which are listed in descending order of importance:

1) Scientific and/or Technical Merit of the Project;
2) Appropriateness of the Proposed Method or Approach;
3) Appropriateness of the management plan.
4) Competency of Researcher's Personnel and Adequacy of Proposed Resources; and
5) Reasonableness and Appropriateness of the Proposed Budget.

The evaluation process will include program policy factors such as the relevance of the proposed research to the agency's programmatic needs. Note that external peer reviewers are selected with regard to both their scientific expertise and the absence of conflict-of-interest issues. Both Federal and non-Federal reviewers may be used, and submission of a proposal constitutes agreement that this is acceptable to the investigator(s) and the submitting institution.

2. Summary of Proposal Contents

- Field Work Proposal (FWP) Format (Reference DOE Order 412.1A) (DOE ONLY)
- Proposal Cover Page
- Table of Contents
- Budget (DOE Form 4620.1) and Budget Explanation
- Abstract (one page)
- Narrative (main technical portion of the proposal, including background/introduction, proposed research and methods, timetable of activities, and responsibilities of key project personnel)
- Literature Cited
- Biographical Sketches

- Description of Facilities and Resources
- Other Support of Investigators
- Appendix (optional)

2.1 Submission Instructions

Have your LAB administrator submit the entire LAB proposal and FWP via Searchable FWP (https://www.osti.gov/fwp). If you have questions about who your LAB administrator is or how to use Searchable FWP, please contact the Searchable FWP Support Center.

Please submit, via Federal Express, a single PDF file of the entire LAB proposal and FWP on a CD along with two hard copies to the address below. This will assist in expediting the review process.

Please send the CD and 2 hard copies via Federal Express to:

Karen Carlson-Brown
Climate and Environmental Sciences Division, SC-23.1
Office of Biological and Environmental Research
Office of Science
19901 Germantown Road
Germantown, MD 20874-1290
ATTN: CSSEF

For further information contact:

Dr. Wanda Ferrell
Program Manager
Regional and Global Climate Modeling
Climate and Environmental Sciences Division
Tel: (301) 903-3281
Email: Wanda.Ferrell@science.doe.gov

3. Detailed Contents of the Proposal

Adherence to type size and line spacing requirements is necessary for several reasons. Small type may also make it difficult for reviewers to read the proposal. Proposals must have 1-inch margins at the top, bottom, and on each side. Type sizes must be at least 11 point. Line spacing is at the discretion of the researcher but there must be no more than 6 lines per vertical inch of text. Pages should be standard 8 ½ inch × 11 inch (or metric A4, i.e., 210 mm × 297 mm).

3.1 Field Work Proposal Format (Reference DOE Order 412.1A) (DOE ONLY)

The Field Work Proposal (FWP) is to be prepared and submitted consistent with policies of the investigator's laboratory and the local DOE Operations Office. Additional information is also requested to allow for scientific/technical merit review.

3.2 Proposal Cover Page

The following proposal cover page information may be placed on plain paper. No form is required.

Title of proposed project

Name of laboratory
Name of principal investigator (PI)
Position title of PI
Mailing address of PI

Telephone of PI
Fax number of PI
Electronic mail address of PI
Name of official signing for laboratory*
Title of official
Fax number of official
Telephone of official
Electronic mail address of official
Requested funding for each year; total request
Use of human subjects in proposed project:

> If activities involving human subjects are not planned at any time during the proposed project period, state “No”; otherwise state “Yes”, provide the IRB Approval date and Assurance of Compliance Number and include all necessary information with the proposal should human subjects be involved.

Use of vertebrate animals in proposed project:

> If activities involving vertebrate animals are not planned at any time during this project, state “No”; otherwise state “Yes” and provide the IACUC Approval date and Animal Welfare Assurance number from NIH and include all necessary information with the proposal.

Signature of PI, date of signature
Signature of official, date of signature*

*The signature certifies that personnel and facilities are available as stated in the proposal, if the project is funded.

3.3 Table of Contents

Provide the initial page number for each of the sections of the proposal. Number pages consecutively at the bottom of each page throughout the proposal. Start each major section at the top of a new page. Do not use unnumbered pages, and do not use suffices, such as 5a, 5b.

3.4 Budget and Budget Explanation

A detailed budget is required for the entire project period and for each fiscal year. It is preferred that DOE’s budget page, Form 4620.1 be used for providing budget information*. Modifications of categories are permissible to comply with institutional practices, for example with regard to overhead costs.

A written justification of each budget item is to follow the budget pages. For personnel this should take the form of a one-sentence statement of the role of the person in the project. Provide a detailed justification of the need for each item of permanent equipment. Explain each of the other direct costs in sufficient detail for reviewers to be able to judge the appropriateness of the amount requested.

Further instructions regarding the budget are given in section 4 of this guide.

* Form 4620.1 is available at web site: http://www.science.doe.gov/grants/budgetform.pdf

3.5 Abstract

Summarize the proposal in one page. Give the project objectives (in broad scientific terms), the approach to be used, and what the research is intended to accomplish. State the hypotheses to be tested (if any). At the top of the abstract provide the name of the lead DOE national Laboratory, project title, names of all the investigators and their institutions, and contact information for the principal investigator, including e-mail address.

3.6 Narrative

(Main technical portion of the proposal, including background/introduction, proposed research and methods, timetable of activities, and responsibilities of key project personnel).

The narrative comprises the research plan for the project. It should contain enough background material in the Introduction, including review of the relevant literature, to demonstrate sufficient knowledge of the state of the science. The major part of the narrative should be devoted to a description and justification of the proposed project, including details of the methods to be used. It should also include a timeline for the major activities of the proposed project, and should indicate which project personnel will be responsible for which activities. It is important that the technical information section provide a complete description of the proposed work, because reviewers are not obliged to read the Appendices.

The proposal must explicitly state how the proposed project will support the accomplishment of the BER climate science LTM.

Since the project is to be done in **collaboration** with other national laboratories, provide information on the participating institution and what part of the project it will carry out. Further information on any such arrangements is to be given in the sections "Budget and Budget Explanation," "Biographical Sketches," and "Description of Facilities and Resources."

3.7 Management Plan

Provide an overview of the organizational structure. This should include where the project resides within the Oak Ridge National Laboratory organization; the leadership structure and how it relates to leadership within the National Laboratory. This section also should describe a plan for internal interactions within ORNL and for interactions with the other national laboratory participants. A staffing and organizational structure chart should be provided. A project manager/project controls individual should be identified and reporting procedures should be defined. The proposal should provide a timeline of specific products that are associated with the four areas of research.

3.8 Literature Cited

Give full bibliographic entries for each publication cited in the narrative. Each reference must include the names of all authors (in the same sequence in which they appear in the publication), the article and journal title, book title, volume number, page numbers, and year of publication. Include only bibliographic citations. Principal investigators should be especially careful to follow scholarly practices in providing citations for source materials relied upon when preparing any section of the proposal.

3.9 Biographical Sketches

This information is required for senior personnel at the institution submitting the proposal and at all subcontracting institutions. The biographical sketch is limited to a maximum of two pages for each investigator and must include:

Education and Training. Undergraduate, graduate and postdoctoral training, provide institution, major/area, degree and year.

Research and Professional Experience. Beginning with the current position list, in chronological order, professional/academic positions with a brief description.

Publications. Provide a list of up to 10 publications most closely related to the proposed project. For each publication, identify the names of all authors (in the same sequence in which they appear in the publication), the article title, book or journal title, volume number, page numbers, year of publication, and website address if available electronically. Patents, copyrights and software systems developed may be provided in addition to or substituted for publications.

Synergistic Activities. List no more than five professional and scholarly activities related to the effort proposed.

To assist in the identification of potential conflicts of interest or bias in the selection of reviewers, the following information must also be provided in each biographical sketch.

> *Collaborators and Co-editors:* A list of all persons in alphabetical order (including their current organizational affiliations) who are currently, or who have been, collaborators or co-authors with the investigator on a research project, book or book article, report, abstract, or paper during the 48 months preceding the submission of the proposal. Also, include those individuals who are currently or have been co-editors of a special issue of a journal, compendium, or conference proceedings during the 24 months preceding the submission of the proposal. Finally, list any individuals who are not listed in the previous categories with whom you are discussing future collaborations. If there are no collaborators or co-editors to report, this should be so indicated.

> *Graduate and Postdoctoral Advisors and Advisees:* A list of the names of the individual's own graduate advisor(s) and principal postdoctoral sponsor(s), and their current organizational affiliations. A list of the names of the individual's graduate students and postdoctoral associates during the past five years, and their current organizational affiliations.

3.10 Description of Facilities and Resources

Facilities to be used for the conduct of the proposed research should be briefly described. Indicate the pertinent capabilities of the institution, including support facilities (such as access to high performance computing capabilities capable of petaflop performance), that will be used during the project. List the most important equipment items already available for the project and their pertinent capabilities. Include this information for each subcontracting institution.

3.11 Other Support of Investigators

Other support is defined as all financial resources, whether Federal, non-Federal, commercial, or institutional, available in direct support of an individual's research endeavors. Information on active and pending other support is required for all senior personnel, including investigators at collaborating institutions to be funded by a subcontract. For each item of other support, give the organization or agency, inclusive dates of the project or proposed project, annual funding, and level of effort (months per year or percentage of the year) devoted to the project.

3.11 Appendix

Information not easily accessible to a reviewer may be included in an appendix. Reviewers are not required to consider information in an appendix, and reviewers may not have time to read extensive appendix materials with the same care they would use with the proposal proper.

The appendix may contain the following items: up to five publications, manuscripts accepted for publication, abstracts, patents, or other printed materials directly relevant to this project, but not generally available to the scientific community; and letters from investigators at other institutions stating their agreement to participate in the project (do not include letters of endorsement of the project).

4. Detailed Instructions for the Budget

(DOE Form 4620.1 "Budget Page" may be used).

4.1 Salaries and Wages

List the names of the principal investigator and other key personnel and the estimated number of person-months for which DOE funding is requested. Proposers should list the number of postdoctoral associates and other professional positions included in the proposal and indicate the number of full-time-equivalent (FTE) person-months and rate of pay (hourly, monthly or annually). For graduate and undergraduate students and all other personnel categories such as secretarial, clerical, technical, etc., show the total number of people needed in each job title and total salaries needed. Salaries requested must be consistent with the institution's regular practices. The budget explanation should define concisely the role of each position in the overall project.

4.2 Equipment

DOE defines equipment as "an item of tangible personal property that has a useful life of more than two years and an acquisition cost of $50,000 or more." Special purpose equipment means equipment which is used only for research, scientific or other technical activities. Items of needed equipment should be individually listed by description and estimated cost, including tax, and adequately justified. Allowable items ordinarily will be limited to scientific equipment that is not already available for the conduct of the work. General purpose office equipment normally will not be considered eligible for support.

4.3 Domestic Travel

The type and extent of travel and its relation to the research should be specified. Funds may be requested for attendance at meetings and conferences, other travel associated with the work and subsistence. In order to qualify for support, attendance at meetings or conferences must enhance the investigator's capability to perform the research, plan extensions of it, or disseminate its results. Consultant's travel costs also may be requested.

4.4 Foreign Travel

Foreign travel is any travel outside Canada and the United States and its territories and possessions. Foreign travel may be approved only if it is directly related to project objectives.

4.5 Other Direct Costs

The budget should itemize other anticipated direct costs not included under the headings above, including materials and supplies, publication costs, computer services, and consultant services (which are discussed below). Other examples are: aircraft rental, space rental at research establishments away from the institution, minor building alterations, service charges, and fabrication of equipment or systems not available off- the-shelf. Reference books and periodicals may be charged to the project only if they are specifically related to the research.

a) **Materials and Supplies**
The budget should indicate in general terms the type of required expendable materials and supplies with their estimated costs. The breakdown should be more detailed when the cost is substantial.

b) **Publication Costs/Page Charges**
The budget may request funds for the costs of preparing and publishing the results of research, including costs of reports, reprints page charges, or other journal costs (except costs for prior or early publication), and necessary illustrations.

c) **Consultant Services**
Anticipated consultant services should be justified and information furnished on each individual's expertise, primary organizational affiliation, daily compensation rate and number of days expected service. Consultant's travel costs should be listed separately under travel in the budget.

d) **Computer Services**
The cost of computer services, including computer-based retrieval of scientific and technical information, may be requested. A justification based on the established computer service rates should be included.

e) **Subcontracts**
Subcontracts should be listed so that they can be properly evaluated. There should be an anticipated cost and an explanation of that cost for each subcontract. The total amount of each subcontract should also appear as a budget item.

4.6 Indirect Costs

Explain the basis for each overhead and indirect cost. Include the current rates.

APPENDIX 2: LETTERS OF SUPPORT

PURDUE
UNIVERSITY

DEPARTMENT OF FORESTRY AND NATURAL RESOURCES
DEPARTMENT OF BIOLOGICAL SCIENCES

Dr. David Bader
Environmental Sciences Division
Oak Ridge National Laboratory
Oak Ridge, TN 37831

Dear Dr. Bader,

This letter is in support of your proposal titled "Climate Science for a Sustainable Energy Future (CSSEF)", being submitted to U.S. Department of Energy, Office of Biological and Environmental Research. I am writing in my capacity as the PI of a recently funded Research Coordination Network (RCN), titled "Integrated Network for Terrestrial Ecosystem Research on Feedbacks to the Atmosphere and ClimatE: Linking experimentalists, ecosystem and Earth system modelers", also known as INTERFACE (support from NSF).

INTERFACE is currently in the first year of a five-year effort to bring together a diverse community of land ecosystem experimentalists, ecosystem modelers, and Earth system modelers. Our funding is primarily directed towards support for a series of meetings and workshops in which specific coordination topics and problems will be addressed and solved. A critical need emerging from a recent INTERFACE-sponsored brainstorming session, held in conjunction with the recent CESM Annual Workshop (June 2010), was for the development of an interface which provides ready access to Earth system models, and more specifically to their land components such as CLM. Specifically, the group saw a need to improve the ability of the Earth system modeling community to engage with the community of researchers performing experimental manipulations of land ecosystems, to facilitate transfer of knowledge back and forth. There is a clear opportunity to leverage the existing INTERFACE connections within the land process research community and INTERFACE resources for workshop support with the land model testbed and data development effort described in your CSSEF proposal.

Specifically, if your proposal is successful, I envision that INTERFACE could provide assistance with connecting experimentalists studying the effects of environmental changes on terrestrial ecosystems with researchers in your effort. For instance, activities that facilitate the development (and later evaluation) of design criteria for a land model testbed might take place in conjunction with INTERFACE-sponsored workshops, which would leverage funding from both groups. Our Steering Committee would be very interested in discussing a variety of models for collaboration in the future.

Wishing you success on your proposal,

Jeffrey Dukes
Assistant Professor

715 WEST STATE STREET WEST LAFAYETTE, IN 47907-2061 EMAIL: JSDUKES@PURDUE.EDU

JUL-29-2010 12:51 12118 FAX 3017130518 P.02/03

UNITED STATES DEPARTMENT OF COMMERCE
National Oceanic and Atmospheric Administration
OFFICE OF OCEANIC AND ATMOSPHERIC RESEARCH
Climate Program Office
1315 East-West Highway, SSMC3, 12th Floor, R/CP
Silver Springs, MD 20910-6233

July 29, 2010

David C. Bader, Deputy Director
Oak Ridge Climate Change Science Institute
Oak Ridge National Laboratory
PO Box 2008
Oak Ridge, TN 37831

Dear Dave,

I've read the draft 'Climate Science for a Sustainable Energy Future (CSSEP)'. It is certainly true that climate simulation and prediction have entered a new and more demanding era. I am very supportive of both the strategy to look two generations past the current CESM and focusing on models with the atmospheric resolution in the 10-15 km range. The link to CESM development cycles should maintain and improve the productive DOE-NCAR model development partnership.

As you know NOAA has embarked on the development of a Climate Service. Delivery of products in support of decision makers is dominated by analysis with state-of-the-art models through model-observations comparison. Although NOAA GFDL has a long-term development path for succeeding generations of Earth System Models, they do not have the ability to accelerate development in anticipation of near term requirements important to decision makers across the spectrum from energy sustainability through water resources to ecosystems, sea level rise, etc.

NOAA has initiated development of a capability to support state-of-the-art approaches and applications of downscaled climate projection information to support regional decision making, including facilitating better connectivity of high resolution data with decision processes and models. A critical element to success will be access to the best climate projections available. The proposed CCSEP would provide rapid evolution of credible projections, improving the utility of products in support of decision makers.

I heartily endorse this proposed effort and hope that a successful result will offer opportunity for close NOAA-DOE collaboration on our closely aligned challenges.

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Sincerely,

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TOTAL P.03

APPENDIX 3: CESM SCIENCE PLAN

CESM

Community Earth System Model

Science Plan: 2009 – 2015

Community Earth System Model

Science Plan: 2009 – 2015

Commissioned by the CESM Scientific Steering Committee:

Peter Gent, NCAR (Chairman)
David Bader, Lawrence Livermore National Laboratory
Gordon Bonan, NCAR
Christopher Bretherton, University of Washington
William Collins, Lawrence Berkeley National Laboratory
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Jay Fein, NSF (ex-officio)

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1) Introduction

Earth System Model development is an ongoing enterprise, with new model versions assembled and released at approximately five-year intervals. Continued development is enabled by new scientific understanding combined with increasing computational capability and capacity. It is generally agreed that the primary directions in the future will be the addition of new processes and components that are absent in current models, and using increased resolution in all components. This Science Plan defines a path to develop model versions that can be used to address societal needs such as predicting climate change on regional space scales and decadal time scales, to evaluate adaptation and mitigation strategies on decadal to centennial time scales, and to identify possible mechanisms for unintended and dramatic abrupt climate changes. As part of this plan, further integration of Earth System Modeling with Integrated Assessment should be continued, using a "system of systems" approach to fully encompass the natural and human systems involved in climate change. The combined Earth System and Integrated Assessment framework permits exploration of energy strategies, and future adaptation and mitigation options. This road map for model development aims to match anticipated improvements in scientific understanding with anticipated advancements in computational capabilities to achieve the maximum benefits of "exascale" computing in 2020.

Substantial progress has been made on incorporating the following new components into the model framework: an interactive carbon cycle, updated atmospheric chemistry component, a version in which the atmosphere component incorporates the whole atmosphere up to the lower mesosphere, rather than just the troposphere, and an early version of a new land ice component. The most widely used description of a model with these capabilities within the climate community is an Earth System Model. For this reason, the Scientific Steering Committee (SSC) decided that, when these components are ready in 2010, the project and supported model should be called the Community Earth System Model (CESM).

Using the CESM to produce decadal projections and predictions on regional spatial scales will require higher resolution components, and the ability to initialize the ocean component in the most appropriate way. Plans are to use 0.5° resolution in the atmosphere component for the initial CESM decadal predictions. As the atmosphere resolution is increased, this highlights the idea of seamless prediction, where the same atmosphere component is used for both weather forecasting and climate simulations. At the least, this requires a common computational core for these two applications. However, increasing resolution is not a panacea to eliminate all the biases in climate model simulations. Thus, continued emphasis in the CESM project must be on the quality of the physical components to simulate coupled phenomena such as the El Nino-Southern Oscillation (ENSO). There needs to be a continued commitment to model-data evaluation to constrain the size of climate feedbacks and the climate sensitivity. Further paleoclimate studies are also necessary to test the CESM in situations very different from the Earth's present climate.

The interactive carbon cycle includes the effects of nitrogen limitation on the land carbon, land use changes due to human activity in the past, a dynamic vegetation component, and an ecosystem-biological module in the ocean component. All previous future projection runs using the CESM have been based on future estimates of the atmospheric concentrations of carbon dioxide. However, the interactive carbon cycle will change to using future estimates of carbon dioxide emissions, rather than concentrations. It will then determine internally how much carbon dioxide is taken up by the land and ocean, and consequently how much stays in the atmosphere. Thus, the interactive carbon cycle model will incorporate the positive feedback due to the carbon cycle, if the land and ocean take up less carbon dioxide in the future than they have in the past.

There are studies which suggest that the ozone levels in the southern hemisphere troposphere are influenced by the dynamics and circulation of the stratosphere. If that is the case, then an atmosphere component that only represents the troposphere cannot predict correctly the future ozone levels in the southern hemisphere, where the "ozone hole" occurs. In order that this process is represented correctly in future climate projections, the atmosphere component needs to incorporate the whole atmosphere up to the lower mesosphere. The CESM has such an atmosphere component called the Whole Atmosphere Community Climate Model (WACCM). The CESM also has an updated chemistry component that can be used to predict the future aerosol pollution in megacities over the next few decades. This relies on a much improved aerosol scheme that has already been incorporated into the atmosphere component. Both of these components are very computationally expensive, but can be used for research work and for a few future climate projection runs.

One of the biggest unknowns about the future climate over the 21st century is how much of the Greenland and Antarctic ice sheets will melt as the climate warms. This has large implications for the future sea level rise, with large consequences for the human population in low lying areas. The CESM has just formed a new Land Ice Working Group, which is now working on a new land ice component. The first version will be applied to the Greenland ice sheet, and will address how much ice will melt into the ocean for a given temperature rise. Subsequent versions will be more comprehensive, and include the interaction between ice shelves and the ocean. Such a model is needed to address the future behavior of the Antarctic ice sheet.

The CESM project is governed by the SSC, which presently has five members from NCAR and seven from the Department of Energy and US University communities. The project receives most of its funding from the Atmospheric Sciences Division at the National Science Foundation and the Office of Biological and Environmental Research at the Department of Energy. The project has oversight from an Advisory Board, which meets annually at the NSF, and reports back to NSF, DOE, and the NCAR Director.

2) Scientific Objectives of the CESM Program

DOE and NSF, as partners in the overall USA Climate Change and Science Program (CCSP), need a core model system for multiple purposes, including future projections of climate change. CESM has participation from a very large community of scientists, and peer-acceptance, which is important to ensure excellence and relevance. Major modeling programs are no longer single Principal Investigator research projects, because of the complexity of the problem and the technical sophistication of the models and computer codes. They are major technology development efforts, and are both shared research tools and major code projects. The CESM community enables access to contributions from multiple sources in an open development process that allows incorporation and testing of a wide range of ideas in a broad spectrum of disciplines. The CESM program also has a mission to foster the creative involvement of University researchers and students in the subject area, and thus contributes to the development of highly trained people for the future. The CESM program is a complement to the other major modeling programs in CCSP that are specifically oriented towards a government mission to provide decision-support information.

The scientific objectives of the CESM program are to:

a) Develop and continuously improve a comprehensive Earth modeling system that is at the forefront of international efforts to understand and predict the behavior of Earth's climate.

b) Use this modeling system to investigate and understand the mechanisms that lead to interdecadal, interannual, and seasonal variability in Earth's climate.

c) Explore the history of Earth's climate through the application of versions of the CESM suitable for paleoclimate simulations.

d) Apply this modeling system to estimate the likely future of Earth's environment, in order to provide information required by governments in support of local, state, national, and international policy determination.

3) History and Accomplishments of the CCSM Project

In 1993, a small group of scientists within the Climate and Global Dynamics Division of NCAR began meeting to discuss the possibility of building a new, comprehensive, coupled climate model. The basic agreement was that the model would be composed of existing component models in use within the division, that these models would be coupled together through a separate module or coupler, and that no flux corrections or flux adjustments would be used to alleviate biases within the coupled system. Coupled model development began in 1994. In 1996, the first coupled simulation was carried out, and this initial simulation showed no indication of the surface climate drift exhibited in all previous coupled simulations carried out by the international community. This was a very significant accomplishment in the science of coupled models, because using a model without flux corrections gives much more confidence about the model's future climate projections. The first Annual Workshop was held in Breckenridge in May 1996, where results from the simulation of a 300-year control run were presented. It was recognized that further development of the CCSM would require a more organized management structure, so the CCSM Scientific Steering Committee (SSC) was formed shortly after the workshop. At this time various working groups were formed to provide forums for model development and application activities. The first version of the Climate System Model, CSM1, was released to the community in June 1996, and a special issue of the Journal of Climate devoted to results from the CSM 1 was published in June 1998.

At this time it was recognized that further development of the model would require expertise in a wide range of disciplines. Also, scientists from the University community and DOE Laboratories were interested in contributing to development of the model. The result was that the project changed its name to the Community Climate System Model, and the DOE became a formal sponsor of the project. The second version of the model, CCSM 2, was released in May 2002. It contained a completely new sea-ice component that was developed from scratch by the Polar Climate Working Group, and completely revised land and ocean components. However, there were several aspects of the model, especially in the atmosphere component, that could be improved on, so it was decided to press ahead quickly to produce a third model version. The CCSM 3 was released in June 2004 in time for the 9th Annual Workshop in Santa Fe, New Mexico. It had further improvements in all the components compared to the CCSM 2. These improvements were again documented in a special issue of the Journal of Climate that contained

26 papers on results from the CCSM 3 that was published in June 2006. In addition, novel software engineering aspects of the CCSM 3 were documented in 13 papers that were published in a special issue of The International Journal of High Performance Computing Applications that appeared in the fall of 2005. This special issue reflects the importance of the software engineering aspects of the CCSM project. It is a huge challenge to keep a code base that works well across a large variety of computer platforms from a personal computer to a very large massively parallel machine, while maintaining a code that can be understood and changed by individual scientists.

The 4th Assessment Report of the Intergovernmental Panel on Climate Change (IPCC) was published in February 2007 to great acclaim, and the IPCC shared the 2007 Nobel Peace Prize. The CCSM project was a major contributor to this report in three ways. First, the CCSM 3 was used to produce control runs, and an ensemble of 20th and 21st Century runs. In fact, the CCSM project contributed more years of integration and results to the AR 4 than any other climate project or center. Second, several scientists heavily involved in the CCSM project were Contributing Lead Authors and Lead Authors on several important chapters, and so made very important contributions to the AR 4. Third, the CCSM community influenced the 4th Assessment significantly through numerous individual research papers using the CCSM that defined the scope of key scientific questions.

There are now a total of twelve Working Groups. The Atmosphere, Ocean, Land and Polar groups develop the physical components of the model, including the sea-ice component. The Biogeochemistry and Chemistry groups develop the carbon and nitrogen cycle and chemistry components. The Climate Variability and Climate Change groups analyze model output from a variety of integrations in order to validate the model variability and to document future climate projections by the model. The Paleoclimate group uses the model to study the climate of past epochs, and the Software Engineering group ensures that the model runs well on a variety of computers, passes many computing tests, etc. Over the past year, two new Working Groups have been formed. The first is the Whole Atmosphere group that both maintains the whole atmosphere version of the CESM and studies the influence of the upper and middle atmosphere on the troposphere. The second is a very new Land Ice group that is producing a component that models the Greenland and Antarctic ice sheets. This aspect of the model is new, but is extremely important if the project is to give realistic estimates of the possible future sea level rise. All the Working Groups meet twice a year, and report back to the SSC. One of the meetings is at the Annual Workshop, which has now been held every year from 1996 through 2009. Most of the Workshops have been held in Breckenridge, Colorado. The SSC and the Advisory Board also hold meetings at the Workshop. The Annual Workshop has become one of the most comprehensive annual climate modeling meetings in the United States. Workshop attendance has grown considerably over the years to more than 300 attendees.

4) Near-term Development of the CCSM 4

Development of the next version of the CCSM started soon after the release of the third version in 2004. Substantial progress had been made by June 2007, so that the SSC decided that an interim version, CCSM 3.5, should be assembled. This happened at the end of September 2007, but the version was not formally released in the sense that it wasn't made publically available and it didn't have the usual documentation. However, it was made available to scientists who were strongly contributing to model development through participation in a Working Group. CCSM 3.5 has numerous changes and improvements, which are briefly documented below, and see Gent et al. (2009).

The core of the Community Atmosphere Model (CAM) version 3.5, changed from the spectral core used in CAM 3 to the Lin-Rood finite volume core, see Lin (2004). Major changes were made to the deep convection scheme by including the effects of deep convection in the momentum equation, see Richter and Rasch (2008), and using a dilute, rather than an undilute, approximation in the plume calculation. These changes resulted in a major improvement in the simulation of ENSO in CCSM 3.5, which is documented in Neale et al. (2008). In CCSM 3, the ENSO frequency was dominated by variability at 2 years, whereas in CCSM 3.5 there is virtually no power at 2 years, and the power is between 3-6 years. In addition, the mean precipitation and double Intertropical Convergence Zone biases in the western tropical Pacific Ocean were considerably reduced, but not eliminated. A freeze-dry modification was added to the low cloud parameterization, which had the effect of reducing the amount of low cloud in the Arctic region. There are 26 vertical levels in CAM 3.5, the same as in CAM 3.

There have also been a number of changes to the ocean component of CCSM 3.5. The near-surface eddy flux parameterization has been modified to be more in line with observations, see Danabasoglu et al. (2008), and the isopycnal diffusivity is a function of space and time, see Danabasoglu and Marshall (2007). The anisotropic horizontal viscosity scheme has been changed in that the Smagorinsky term has been removed, and viscosity is now substantially smaller near the equator, see Jochum et al. (2008). The vertical mixing terms now have a term that is proportional to the tidal energy, and the advection scheme has been changed from the third-order upwind to a flux-limited Lax-Wendroff type scheme that is less diffusive. There are now 60 levels in the vertical, as opposed to 40 in CCSM 3.

The Community Land Model (CLM), version 3.5 is documented in Oleson et al. (2008) and Stockli et al. (2008). There were changes to many parts of the model hydrology, such as the surface runoff, the groundwater scheme, the frozen soil scheme, and a soil evaporation resistance was added. Other new features are a revised canopy integration, canopy interception scaling, and a plant functional type dependency on the soil moisture stress function. CLM 3.5 has a much improved representation of evapotransportation and the annual cycle of water storage, for example.

The sea ice component in CCSM 3.5 moved to the Community Ice Code, version 4.0 as its base code, which is maintained at the Los Alamos National Laboratory. This brought in improved treatments of ice ridging and snow on top of the ice. In addition, the much improved radiative transfer scheme of Briegleb and Light (2007) and a new melt pond parameterization were included.

Since the assembly of version 3.5, there have been further developments in all four physical components, but especially in the atmosphere. The Atmosphere Model Working Group has been implementing and evaluating four major changes to the CAM 3.5. The first is changing the radiation computation to use the RRTMG scheme, and the second is including the cloud microphysics scheme of (Morrison and Gettelman, 2008). The third is the modal aerosol scheme of Ghan and Liu that has been refined to use only three modes. This scheme is needed if the CCSM 4 is to include the indirect effects of aerosols. The fourth major change is to include the boundary layer parameterization and shallow convection scheme of Bretherton and Park. The Ocean Model Working Group has been implementing a new scheme to determine the effects of overflows over deep sills in the ocean, and a new parameterization of the effects of submesoscale eddies on the ocean mixed layer of Fox-Kemper et al., (2009). The Land Model Working Group has built on and refined the improvements in CLM 3.5, and the Polar Working Group has worked on further improvements to the sea-ice component, including using more realistic albedo values.

Assembly of the CCSM 4 will take place over the first part of 2009. First, a 1850 Control run that goes for several hundred years and is well balanced at the top of the atmosphere is required. Then, a 20th Century run from 1850 to 2005 has to be completed that gives a realistic simulation of the true climate over this period. When this is completed, the standard resolution version of the CCSM 4 will be defined. However, a half degree resolution version of the land and atmosphere components is needed, that will be used to make decadal climate predictions for the IPCC AR5. In addition, a low resolution CCSM 4 version is needed for Paleoclimate studies. The standard resolution version of the CCSM 4 should be ready by June, 2009, and will probably be released for public web download later in 2009. The half degree and low resolution versions should be ready later in 2009.

Once the new CAM 4 is defined, then other Working Groups can begin to finalize their components. In particular, the Chemistry and Whole Atmosphere components rely very heavily on the atmosphere component, and to a somewhat lesser extent, so do the carbon cycle/biogeochemistry component. The last additional component is the new land-ice model for ice sheets. These components will not be finished until later in 2009, and possibly released early in 2010. When this second release occurs, the CCSM 4 will become the CESM 1.

5) Scientific Questions to be Addressed

a) Interaction of the Carbon Cycle, Ecosystems and Climate

Land and ocean life can influence climate through a variety of biogeophysical and biogeochemical pathways. Interactions between climate and ecosystem processes, especially in response to human modification of ecosystems and atmospheric carbon dioxide (CO_2) growth, will likely produce a rich array of climate forcings and feedbacks that could either amplify or diminish climate change. Biota will also modulate regional patterns of climate change. Ecosystems are the focus of many carbon sequestration approaches for mitigating climate change, and are the central elements of potential climate impacts associated with food security, water resources, human health and biodiversity. However, the magnitude of these climate-biota interactions, and in some cases even the sign, are not well constrained, and are critical scientific unknowns affecting the skill of future climate projections.

Terrestrial vegetation alters the albedo of the land surface and modulates the exchange of momentum, sensible and latent heat, and water vapor across the land-atmosphere interface. Current understanding suggests negative biogeophysical climate forcing (cooling) associated with historical and future expansion of agricultural land in the mid-latitudes and positive climate forcing (warming) due to tropical deforestation. Open research questions include the extent and effects of past and present land-use change e.g., transition of natural ecosystems to agriculture and managed forestry; shifts in managed systems due to climate trends, bioenergy, and carbon sequestration; and expansion of urban and suburban areas, and the poleward migration of natural ecosystems such as the expansion of shrubs into Arctic tundra ecosystems. In the ocean, phytoplankton affect the absorption of sunlight in the upper ocean, and thus sea surface temperature.

Biogeochemical roles within the Earth System are numerous. Biota modulate atmospheric composition for a variety of constituents: atmospheric greenhouse gases such as carbon dioxide, methane, and nitrous oxide; aerosol precursors such as biomass burning and organic sulfur; and trace gases essential to the atmospheric oxidation state. Human emissions of CO_2 are the single largest component of present-day climate change and the contribution of CO_2 will grow over the next several decades, or longer, as CO_2 emissions increase with population and economic growth. At present only about half of anthropogenic carbon remains in the atmosphere to drive climate change; the remainder is removed in about equal amounts by the land biosphere and the oceans. The physical mechanisms governing the ocean carbon sink are relatively well understood, but the effectiveness of the future ocean sink is expected to decline due to warming and altered circulation. Models and some recent observations suggest that reduced CO_2 uptake may already be occurring in the Southern Ocean.

Current research suggests that, on balance, terrestrial ecosystems are at present a net sink for CO_2, but this conclusion masks considerable complexity and uncertainty with respect to future behavior. The paradigm captured in the present generation of models is that CO_2 fertilization enhances terrestrial plant productivity, offset by decreased productivity and increased soil carbon loss with warming and soil drying. This conceptual framework neglects nutrient effects, however. The availability of nitrogen, as well as other biogeochemical cycles, e.g., phosphorus, alters the magnitude, and possibly the sign, of the carbon cycle-climate feedback. Additional feedbacks associated with ozone deposition and methane emission will undoubtedly further alter the magnitude of the biogeochemical-climate feedbacks. Climate-carbon models indicate that the land carbon sink may be unstable under future climate change, leading to a potentially large positive feedback. On centennial timescales, climate change may alter the large-scale distribution of natural biomes over the planet, with significant impacts on carbon storage, surface albedo and the water cycle. Human activities play a very direct, and often unaccounted for, role in terrestrial ecosystem dynamics. Deforestation and other land use changes result in a CO_2 flux to the atmosphere, as high-carbon forests are turned into comparatively low-carbon pastures and croplands. This process is now occurring mainly in the tropics, and is countered to an unknown extent by regrowth on abandoned farm and pastureland in the extratropics. The ambiguities in the mechanisms controlling the land carbon sink and their climate sensitivities translate into large uncertainties in future atmospheric CO_2 trajectories and climate change rates; uncertainties that need to be resolved to support carbon mitigation policies.

b) Decadal Climate Projections and Forecasts

Today, there is tremendous societal, as well as scientific, interest in how climate will change over the next several decades. In response, the CESM is moving forward to execute decadal climate projections and forecasts. A list of these projections and forecasts for the 5th Assessment Report of the IPCC has now been assembled. They include a series of 10 year hindcasts and prediction ensembles, some of which are extended for 30 years, including forecasts from 2006 to 2035. Such regional scale simulations will require an ensemble of at least ten runs using finer resolution components, and with the inclusion of simple chemistry, aerosols, and dynamic vegetation modules.

One very interesting and extremely important question is: Does it make a significant difference if the CESM is initialized to the actual climate at the start of the run? Exactly how to initialize the CESM is a major challenge, and one that other climate groups around the world are wrestling with as well. At a minimum, it will require data assimilation into the ocean component, and possibly sea ice extent in the Arctic. Does the CCSM need to have the correct state of the tropical Pacific and ENSO, and the North Atlantic meridional overturning circulation in order to produce a realistic decadal forecast for 2006-2035? There are many other data assimilation issues; for instance how to initialize all the model components around the modes of coupled variability intrinsic to the model.

There are some advantages to these decadal projections and forecasts. First, they are relatively short, so the atmosphere and land components can be run at higher resolution than previously used for IPCC scenario runs. An initial run using half degree resolution in the atmosphere and land components of the CCSM has shown that the sea surface temperature errors in the upwelling regions off the west coasts of North and South America, and off the west coast of Southern Africa are reduced by more than 50% compared to a comparable run using two degree resolution in the atmosphere and land, see Gent et al. (2009). Second, most of the climate change signal is already committed up until 2035, so these forecasts are much less dependent on the uncertainty in future forcing scenarios used to drive them than the traditional longer runs going out to 2100. The rationale for these decadal projections and forecasts is to produce regional climate information for the near future that is more relevant to decision makers.

There are many scientific questions to be addressed and answered better than previously:

1. The runs with and without data assimilation could be used to address the predictability of the climate system on decadal timescales. Also, the evolution of model systematic errors on shorter timescales might give insight into the mechanisms associated with these errors.

2. The decadal projections are a stimulus for a variety of multi-scale modeling activities, such as very high resolution one-way downscaling over the U.S.A. This could be used to examine implications for hydrology and water supplies, such as snow pack and runoff in the west, which is controlled by local mountainous topography.

3. Changes in extremes, such as extended heat waves, floods, droughts and in Atlantic hurricane frequency and intensity can be examined in these runs.

4. With the atmospheric chemistry component included, there will be simulations of the future air pollution, such as aerosols and ozone, in major urban areas and mega-cities.

5. Higher land resolution would also permit simulation of different classes of permafrost, and their different susceptibilities to, and interactions with, future climate change.

6. This type of decadal projection would emphasize human-induced changes in land use, because the dynamic vegetation module in the CESM land component would be active.

c) Interaction of Aerosols and Climate

Aerosols affect the climate in a multitude of ways. They directly reflect and absorb solar radiation in the atmosphere, altering the vertical distribution of short-wave radiation available to the climate system. Aerosols also act as cloud condensation and ice nuclei and regulate cloud properties, which strongly alter the short-wave and long-wave radiation budgets of Earth. Increased numbers of cloud condensation nuclei can produce more of the smaller cloud droplets, which increases a cloud's optical depth. Production of these smaller cloud droplets also suppresses the growth of droplets into larger sizes that precipitate out of the cloud, thus leading to clouds with more condensate and/or longer lifetimes. Increased numbers of ice nuclei can accelerate precipitation from clouds, reducing the cloud liquid water content and lifetime. In addition, absorption of solar radiation by aerosol particles in clouds can reduce the relative humidity and evaporate cloud water. All of these changes lead to changes in the cloud's radiative effects on the Earth's energy budget. Quantifying the anthropogenic aerosol impact on climate is important for isolating human impacts on climate change from natural variability.

The aerosol lifecycle is influenced by climate in several important ways. Emissions of carbonaceous particles from fires change as the climate changes. Emissions of aerosol precursor gases, such as dimethyl sulfate from the ocean and volatile organic carbon from trees, also depend on climate change. Climate-induced changes in the hydrologic cycle can affect aqueous-phase chemical production of sulfate, gas phase photolytic reactions, and removal of aerosol from the atmosphere by precipitation. Deposition of aerosol particles to the surface can reduce the albedo of snow and ice, thereby accelerating snowmelt and icemelt and further reducing the surface and planetary albedo. Deposition of nutrients in particles can enhance the productivity of the land and ocean, and hence influence the carbon cycle, while deposition of acids can reduce the productivity. Emissions of anthropogenic aerosol particles and aerosol precursor gases change as human activities change. Changes in energy technology change emissions of sulfur dioxide. Changes in land use change emissions of carbonaceous aerosol and soil dust.

It is clear that aerosols provide an effective link among a number of components of the Earth's climate system, where they connect the physical, chemical, biogeochemical and human components of the system. Representing all of these interactions requires a size-resolved and speciated representation of the aerosol. All major aerosol components (as a minimum, sulfate, sea salt, dust, organic carbon, black carbon), both natural and anthropogenic, must be treated. A comprehensive representation of the aerosol would be too expensive for many CESM applications, but the modal aerosol model developed for CCSM4 provides a framework that satisfies many of these requirements. The number, as well as mass, of each of three modes is predicted, with multiple components internally mixed within each mode. Parameterizations of all important aerosol processes are included, although the treatment of some processes, new particle formation, formation of secondary organic aerosol, are highly uncertain. Extensions to speciate dust are needed for applications to ice crystal nucleation and ocean fertilization.

d) Interaction of Chemistry and Climate

Changes in the distribution of large population centers are expected to occur over the next decades, with more megacities (population over 10 million) present in developing countries. These represent large "point" sources of pollutant that will lead to significant regional pollution degradation and possibly impacts on regional meteorology and climate. Some of those issues will be tackled under the IPCC AR5 decadal prediction experiments. Beyond those pioneering exercises, this type of regional problem will be particularly suited to an interaction between global and regional chemistry-climate models.

Through the newly developed capability of representing size distribution of aerosols, using the newly implemented modal scheme, CESM is now in position to explore in a more realistic fashion interactions between clouds and aerosols. While many studies can be performed in this framework, there is evidence that the chemical composition of aerosols is a critical element in their ability to act as cloud condensation nuclei. Better representation of the chemistry happening at the surface and inside the aerosols will be needed to ensure the correct representation of the water uptake of aerosols. To benefit from field experiments, this research area will require an ability of the model to perform simulations at high resolution and with large numbers of chemical constituents, thereby extending the on-going research in regional chemistry modeling.

There is increasing evidence that recent changes in atmospheric composition (especially of ozone) have lead to significant perturbations to the temperature distribution. As a corollary, trends in upper-tropospheric and lower-stratospheric climate (width of the tropopause, position of the zonal jets) have been observed, with potential impact on the position of the ITCZ and associated precipitation. The important question is to identify the specific roles of chemistry (through changes in emissions for example) and climate in explaining those trends. This is only one example in a large number of potential studies of interaction between climate (troposphere and stratosphere) and atmospheric composition, especially in relation to IPCC AR5.

Beyond the potential role of CO_2 on vegetation growth, pollution (mostly through ozone and nitrogen deposition) can lead to significant degradation of the ability of plants to grow. This type of problem requires a sizeable increase in the complexity in the representation of the interaction between plants (leaf uptake) and atmospheric chemistry; among other things, this could require a representation of chemistry in the canopy. In addition, recent field studies have highlighted the possible limitation of biogenic emissions (isoprene and monoterpenes) by CO_2, with the overall result of a decrease of the impact of temperature in a high CO_2 world. This can then be extrapolated to the cold climate of the Last Glacial Maximum where biogenic emissions would then increase. This has large implications on the tropospheric OH budget and methane lifetimes.

The Polar Regions are experiencing very significant modifications to their sea-ice distribution, especially in the Northern Hemisphere. Widespread surface (and lower troposphere) ozone depletion episodes (related to halogen chemistry similar to the one occurring in the stratosphere) are observed every winter and spring; these phenomena are not yet fully understood, but there is evidence that they happen through chemistry in the changing snow/ice surface. This halogen chemistry (bromine, chlorine and iodine) is actually present over most of the globe, and needs to be studied more as it reveals interactions between ozone and biogenic (planktonic) emissions from the ocean.

e) Role of the Middle Atmosphere in Climate

The role of the middle atmosphere in climate change is currently an open question. Changes in the propagation characteristics of planetary waves in the stratosphere appear to play a role both in stratospheric climate, via dynamical and chemical interactions that affect ozone concentration, and in tropospheric climate by influencing phenomena such as the Arctic and Antarctic

Oscillations (Thompson et al., 2005; Gillett and Thompson, 2003; Baldwin and Dunkerton, 2001; Son et al., 2008). The dynamics of the stratosphere are dominated by the interaction of dynamical forcing due to waves propagating upward from the troposphere and radiative forcing by solar heating due to ozone. Upward-propagating planetary waves affect the stratosphere directly. Small-scale gravity waves can deposit momentum in the stratosphere itself, or in the mesosphere, where they affect the stratosphere through "downward control." In order to understand the climate role of the stratosphere, it is necessary to model the coupled variability of dynamics and ozone.

The expected cooling in the stratosphere due to increasing CO_2 concentrations in the atmosphere is much larger than the expected increase in surface and tropospheric temperatures. This follows from the fundamental physics of radiative transfer, and is independent of the model used or the magnitude of water vapor feedbacks. Because ozone chemistry is temperature dependent, changes in stratospheric temperature will produce changes in stratospheric ozone, independent of any changes in circulation or sources of other chemical compounds. Of course, changes in chemical species that affect ozone chemistry also influence stratospheric climate, as noted above. Conventional climate models do not resolve the stratosphere adequately, and do not include feedbacks between ozone and dynamics; a deficiency that needs to be corrected.

Several studies have hypothesized that climate variability over the last several centuries is correlated with long-term variations in solar irradiance. There has also been considerable discussion of observed correlations between the 11-year solar cycle and tropospheric temperature and geopotential. However, the total solar irradiance variations do not appear to be large enough to force the observed climate variability in existing models. The radiative transfer codes in current climate models generally do not include wavelengths shorter than 200 nm, because these are almost entirely absorbed above the top boundary of these models. Nevertheless, solar irradiance variations at shorter wavelengths may influence the troposphere and surface climate indirectly, through changes in the stratospheric ozone distribution and circulation. Addressing this question requires models that extend through the mesosphere and include interactions among ultra-violet radiation, ozone chemistry and dynamics (Thompson and Solomon, 2002).

Research on the role of the middle atmosphere in climate and the effects of solar variability at short wavelengths requires a model that extends from the surface through the mesosphere, including interactive ozone chemistry. These requirements are among the goals of the Whole Atmosphere Community Climate Model (WACCM) project, which is motivated by an appreciation of the importance of coupling between different atmospheric regions, and the necessity of studying dynamical and chemical processes interactively and comprehensively. WACCM is built upon the software framework of CESM, in order to benefit from the development of the atmospheric component of the CESM, and the diagnostic infrastructure that exists for that model. However, there are specific needs that are crucial for successful coupling of the troposphere with the middle atmosphere that place constraints on the performance of the atmospheric component of CESM. One example is the requirement that the tropical tropopause in the atmosphere not be too cold compared to observations.

f) Role of Ice Sheets, Sea Ice and Land in Abrupt Climate Change

The climate record shows evidence of rapid and extreme temperature change, sometimes in as little as a decade. An abrupt climate change is thought to occur when the climate system passes a threshold, so that a small perturbation can trigger a large response. Examples of threshold events include iceberg and floodwater outbursts in the North Atlantic that are seen in proxy data, and are associated with the disintegration of the Laurentide ice sheet. The large input of fresh water may have in turn rapidly altered ocean circulation and influenced ocean heat transport. However, evidence for such outbursts preceding rapid climate changes remains uncertain. Furthermore, smaller abrupt changes have been identified during interglacial times as well, so mechanisms in the absence of ice sheets also must be possible.

The mechanisms that cause abrupt changes are not fully understood, and there is general agreement that climate models do not properly represent them. The possibility that an abrupt change will occur in the future due to anthropogenic influences makes the need to understand better their mechanisms an essential element of projections of future climate. Climate models could be used both to identify mechanisms and to estimate their future impacts.

The following candidate processes are thought to be important for abrupt climate change and may require either refinements to existing parameterizations or additions to the model:

- deep water formation
- shelf processes
- fresh water runoff, storage/recycling, atmospheric moisture transport
- sea ice processes
- ice sheet processes
- atmospheric chemistry

g) Bounding Future Climate Scenarios

The best estimate from observations is that over the past 20 years, about half the rise in global sea level has been due to the thermal expansion of the ocean and half due to the increase in ocean volume because of melting land glaciers and ice caps. However, there are growing concerns that both the Greenland and West Antarctic ice sheets are beginning to melt more quickly as the Earth's climate warms (Shepherd and Wingham, 2007). There is evidence that the Greenland ice cap is melting considerably more than it is accumulating over the current decade (Steffen et al. 2004; Hanna et al. 2008). Also over the last decade, several small ice shelves have collapsed in both Greenland and Antarctica. Observations show that the glaciers behind these ice shelves are now flowing much faster than before (Joughin et al. 2003; Scambos et al. 2004; Rignot and Kanagaratnam 2006), which is also increasing the flow of fresh water into the global ocean. It has been suggested that, if the Earth's temperature warms by more than 3°C, then the Greenland ice sheet will become unstable, and will completely melt over the next few centuries. It has also been suggested that this process will be irreversible, even if the Earth's temperature subsequently cools. Total melting of the Greenland ice sheet will increase the global sea level by nearly 7 meters.

The projections of future sea level rise over the 21st century in the IPCC 4th Assessment Report did not take into account the possible increase in melting rates of the Greenland and Antarctic ice sheets. The reason was that the range of melting rate increase was not well bounded, but this implies that the AR4 estimate of sea level rise is almost certainly an underestimate. The CESM project plans to produce a more realistic estimate of the possible sea level rise over the 21st century. To do this, a land ice sheet component is presently being incorporated into the CESM framework. This work is being led by William Lipscomb of the Los Alamos National

Laboratory, with some colleagues from around the US University community. The first version will allow estimates of the future melting rate of the Greenland ice sheet, which affects both sea level rise and the ocean circulation. Additional fresh water deposited into the high-latitude North Atlantic Ocean may further slow down the meridional overturning circulation in the future. Subsequent enhanced versions of the new land ice component will model the interaction between ice shelves and the ocean, and the subsequent acceleration of glaciers behind the ice shelves.

Another possible large positive feedback to the Earth's climate system will occur if the future warming instigates a significant increase in the amount of methane emissions from the northern high-latitudes as Arctic permafrost thaws. Methane is about 25 times more effective as a greenhouse gas than carbon dioxide. It is rather difficult to estimate how much methane emissions might increase. However, there is some concern that it is already happening with observations indicating potentially widespread permafrost warming and thawing, and more limited evidence of associated methane release in parts of Arctic Canada and Siberia. Initial efforts to augment the CESM to address the issue of future northern high-latitude methane emissions have focused on improving the representation of permafrost dynamics (Lawrence et al., 2008). Work is underway to include a global natural methane emissions module, and a dynamic global wetland module into the CESM land component. This will enable the CESM to assess how northern, and global, methane emissions will respond to various climate forcings, and to bound the possibly serious impact of this effect over the 21st century.

h) Simulating Paleoclimates

Studying past climates provides a powerful resource for improving our understanding of the forcings and feedbacks that determine the state of the climate system on the time scale of centuries to millions of years. Paleoclimate simulations also act as means to integrate Earth as a system, because on these time scales physical, chemical, biogeochemical and ecological processes are integrally coupled. Thus, investigations of paleoclimate require the development of a comprehensive Earth System Model.

Studying past climates also provides valuable information on key processes that operate in warm climate regimes. It is estimated that by the end of this century Earth will experience a radiative forcing of somewhere between 5 to 10 Wm^{-2} due to increases in anthropogenic atmospheric carbon dioxide. Earth has not experienced this magnitude of greenhouse forcing for tens of millions of years. Thus, by simulating past warm climates, the CESM will gain a better understanding of the important Earth system processes that will operate throughout this century. Past climate records also provide evidence for abrupt transitions in the climate system. Paleoclimate simulations can provide important information on the possible mechanisms for such abrupt transitions. Thus, paleoclimate simulations provide a unique opportunity to provide essential information on the future of Earth’s climate.

One metric of success of a new paleoclimate CESM will be to predict the glacial-interglacial Earth system, including climate, ice, carbon cycle, chemistry, and ecosystem, forcing the model only with the insolation variations of the Milankovitch orbital cycles. A second metric of success will be the ability to define the sequence of processes that led to the great mass extinction events in Earth history.

The CESM is a very valuable tool for providing a global perspective for individual ice core measurements and to test hypotheses proposed to explain changes seen in paleoclimate records. Important scientific findings from current CCSM3 climate simulations include: latest Permian (~250 million years ago) simulations confirming the hypothesis that enhanced CO_2 greenhouse warming led to global ocean anoxia, and Last Interglacial (~130 thousand years ago) simulations indicating that Arctic warming comparable to projections over the next few centuries resulted in a smaller and steeper Greenland Ice Sheet.

i) Role of Ocean Mesoscale Eddies in Climate

The ocean interacts with other components of the climate system through the direct influence of sea surface temperature (SST) on the atmosphere, by transporting energy, water, and material around the globe, and by sequestering dissolved gases such as CO_2 in the interior out of contact with the atmosphere. Ocean mesoscale eddies and fronts play a role in each of these processes. The majority of the kinetic energy in the ocean exists at these scales, yet they are substantially smaller than can be explicitly resolved by the standard version of the CESM ocean component. A central problem in oceanography is to quantify the processes through which eddies and fronts influence the larger scale climate, and to represent these processes through parameterization in climate models.

While parameterizations of the effect of mesoscale eddies on the distribution of scalar properties continue to advance (e.g. Danabasoglu and Marshall, 2007), there remain significant gaps in our understanding, aspects that remain unrepresented, and biases in resulting property fluxes. Examples of processes that are not currently represented by mesoscale eddy parameterizations include: the interaction of eddies with inertia-gravity waves, the generation of recirculation gyres adjacent to western boundary currents (Nakano et al., 2008), and the forcing of zonal jet structures in the open ocean (Richards et al., 2006). Vertical motion in mesoscale eddies has also been shown to modify substantially primary productivity of oligotrophic marine ecosystems (McGillicuddy et al., 1998). Parameterizations that depict eddies exclusively as a mixing process cannot represent this nutrient transport mechanism.

Newly available high-resolution remote sensing products for ocean winds, SST, and surface currents have revealed a strong positive correlation between mesoscale SST variability and the surface wind field and heat flux out of the ocean; an indication that the ocean is forcing the atmosphere at these scales (Chelton et al., 2004). These frontal scale influences have been shown to extend out of the surface boundary layer into the troposphere (Minobe et al., 2008), providing a mechanism for scale interaction between the ocean mesoscale and the planetary scale atmospheric circulation. These effects are not represented in models that lack the resolution to explicitly resolve ocean SST fronts.

In order to improve our understanding of ocean mesoscale processes in the global climate, and to progress towards refining existing eddy parameterizations, will require a version of the CESM in which these oceanic scales are explicitly resolved. A suite of simulations in ocean-alone and fully coupled mode is needed to investigate the range of scientific questions outlined above. Recent simulations with basin-scale (Bryan et al., 2007) and global (Maltrud and McClean, 2005) ocean models suggest that a horizontal resolution of 10 km or less is necessary to adequately simulate both the intense western boundary currents and the mesoscale eddies. Prototype CESM experiments with a version of the ocean component configured similarly to the stand-alone ocean model used in (Maltrud and McClean 2005) have recently been carried out. In order to bring this model to the stage that long-term climate experiments are feasible, model developments in physical parameterizations and computational science are required.

Beyond a simple increase of resolution of the present model, CESM will need to continue to explore the sensitivity of eddy resolving solutions to subgrid-scale parameterizations. Despite the fact that mesoscale eddies will be explicitly resolved, adiabatic closure schemes may still be required (Roberts and Marshall, 1998). As yet, no practical scheme has been implemented. Significant interaction between mesoscale eddies and both interior and boundary layer diapycnal processes is expected. In particular, the energy cascade from the mesoscale to the submesocale remains unresolved, and will require further development of the eddy-mixed layer interaction parameterization currently used in the CESM ocean component at coarser resolutions (Fox-Kemper et al., 2009).

The increase in resolution from 100 km to 10 km represents an increase in computational cost of approximately 1000 over the current CCSM ocean component, and will require access to the very highest performance computational systems available. This requires that the model must scale to tens of thousands of processors. Efficient model execution on these systems demands highly scalable implementations of every phase of the code from local communication to global operations. Strong guidance from, and collaborations with, computational science researchers familiar with state-of-the-art computer architectures will be required.

j) Interaction with Integrated Assessment Modeling

The identification and evaluation of climate change response options, including both mitigation and adaptation, requires carrying out integrated analyses involving the physical climate system and the ecological and socio-economic systems with which it interacts. Stronger linkages between the CESM and the integrated assessment modeling (IAM) community offer a new means of bringing such integrated research to bear on pressing questions regarding possible responses to the challenge of climate change. IAMs link quantitative models of socioeconomic and biophysical components of climate change, and apply them to policy-relevant questions. Historically, IAMs have incorporated highly simplified representations of the climate system, and the interaction between the IAM and earth system modeling community has been limited. More recently, however, interest in exploring the potential of linking IAMs with earth system models has grown, stimulated in part by a new, IPCC-catalyzed scenario process that includes interactions between these communities, and will play a key role in generating integrated scenario analyses in the run-up to the IPCC Fifth Assessment Report.

Activities related to CESM that could promote interaction with the IAM community include a range of options, from incremental to ambitious, internal NCAR interactions to collaboration with the wider IAM community, and indirect exchanges to direct model coupling. Possibilities include:

Intensified interaction (e.g., through regular joint workshops) to ensure that IAMs produce inputs most useful to driving CESM simulations, and that CESM produces outputs most useful to IAMs and impact assessment researchers. First steps toward such interactions are occurring through the development of the Representative Concentration Pathways (RCPs) at the core of the new scenario process for AR5. Making CESM outputs more useful to IA could imply, for example, additional emphasis on statistical and conservative downscaling of physical model outputs, and/or high resolution simulations.

- Collaboration with IAM groups on joint research projects and assessments, in which questions arising from the IAM community can help prioritize CESM research directions and identify interesting scenarios to explore. A recent example is provided by a small internal NCAR project on "overshoot" scenarios, which play a key role in IAM analyses of achieving long-term climate change policy goals, and point to a need to assess how the climate system may respond to declining levels of radiative forcing.

- Develop a framework for linking IAMs to biophysical models of the land surface. Interactions at the land surface provide the most immediate interface between human activity and biophysical systems. However, linkage between IAMs and ESMs are difficult to make given differences in spatial scales, categories of land use and cover, ecosystem types, treatment of water systems, etc. A concerted effort could create a focal point within the U.S. for the integration of ecology, hydrology, biogeochemistry, and socioeconomic drivers of land use change into climate science. Such a framework would greatly facilitate the linkage of CESM to IAM models, and greatly improve the ability to conduct climate change impacts, adaptation, and mitigation research related to land use.

- Development of a framework for linking integrated assessment models with CESM more broadly. Such an effort would benefit from the computational resources and modeling expertise within CESM, and make it a leading project in linkages between physical modeling, integrated assessment modeling and quantitative assessment of the impacts of climate change. It would also provide a community modeling platform that was more useful to a wider range of users, including external IAM groups wanting to link their own model to CESM. For this reason, the activity should allow for a variety of different approaches and Integrated Assessment models.

6) Long-term Development of the CESM

a) Future High Resolution Atmospheric Components

In order to simulate more accurately the means and extremes of regional climate, future generations of CESM will have higher resolution atmospheric components, but their development will require significant changes in the numerical algorithms for the dynamics, the grid structure and, ultimately, in the dynamical formulation. When thinking of model resolution, it is necessary to distinguish resolution from grid spacing. With spectral models based on spherical harmonics, the resolution is defined by the wave number truncation with a transformed grid spacing that is typically 3-4 times smaller than the most highly resolved feature. Similarly, for finite difference and finite volume approaches, the resolution is typically a factor of four coarser than the grid resolution, as this is the smallest feature that can be simulated with fidelity by these methods. The current CAM4 production version uses a grid spacing of approximately 100 km, which results in an equivalent resolution for a spectral model of T85, although experimental versions are in use with resolutions two and four times greater.

Climate models benefit greatly from atmospheric general circulation model (GCM) development by the global numerical weather prediction (NWP) centers. In general, a state-of-the-science climate model is a factor of 3 to 10 behind current NWP models in terms of resolution because of the increased simulation times and the inclusion of processes that are important to climate, but are inconsequential to influence 10-day predictions. The global weather prediction model used today by the European Center for Medium Range Weather Forecasting (ECMWF) produces 10-day forecasts twice per day using a T799 spectral truncation. The ECMWF employs their very high resolution system to accurately simulate severe weather phenomena, such as localized intense rain or wind areas that are often embedded in larger weather systems, and circulations tied to small-scale terrain or coastlines. The global prediction skill of their model is also improved because the energy transfer among the smaller scales is better resolved. The next generations of CESM should strive for NWP resolution in climate simulations. In the longer term, research into cloud resolving global models, coupled with "Exascale" computing power is expected to lead to climate models that can explicitly resolve clouds and convection, while simultaneously satisfying the global energy and mass constraints to produce accurate climate simulations.

Developing modern climate and weather prediction models requires enormous human effort as many interacting physical processes need to be faithfully represented. Increasingly, we are making weather forecasts with climate models to more efficiently test its parameterizations. Conversely, we are making long simulations with weather prediction models for medium-range forecasting and regional climate modeling. Conceptually, climate and weather forecast models could use unified dynamics and physical parameterizations. This unified model paradigm is being effectively employed at ECMWF and United Kingdom Meteorological Office (UKMO), which now have two of the world's best-performing weather and climate models. The CAM development strategy should adopt this paradigm to the extent practical, while always acknowledging that priority is given to producing the best global climate simulations. An important first step is developing a global climate model with resolution comparable to the best global NWP models in use today, such as those at ECMWF and the UKMO. To the extent possible, CAM development should proceed in close collaboration with NWP modeling groups, particularly the Weather and Research Forecasting (WRF) community. For example, substantial cooperation is anticipated between CAM and WRF developers on evaluating formulations for global nonhydrostatic dynamical cores and grids for future generations of both models.

Development of future higher resolution versions must anticipate and integrate progress in numerical algorithms, programming models and computer architectures (see section 6h). Critical to successful development is an open and thorough testing of competing ideas for the next generations of high resolution atmospheric GCMs. For example, several alternative grids and numerical approaches were explored at the NCAR ASP 2008 Summer Colloquium on Numerical Techniques for Global Atmospheric Models. Although a number of model tests have been developed and applied over the years, CESM should define a priori a full testing hierarchy to guide the development stream (Jablonowski et al, 2008). In particular, the Held-Suarez, aqua-planet and full twenty-year AMIP tests should be applied, in order, with a complete evaluation of each to determine the acceptability of new dynamical cores, model formulations or grids. Furthermore, the model must maintain the mass and energy conservation constraints required to perform century and longer simulations.

CAM5 - 2012

A logical next step for CAM will be developing a next generation dynamical core using the existing hydrostatic model formulation on an isotropic grid, potentially with new algorithmic approach and numerical methods. The target resolution for the model would be close to the limits imposed by the hydrostatic formulation and the scale limits of sub-grid scale parameterizations, which is a grid spacing of approximately 10 km. Possible grids include, but are not limited to, the geodesic grid used by the CSU group and the German weather service, and the cubed-sphere grid used by Japanese groups and GFDL. Potential algorithmic options include the SEAM/HOMME spectral element dynamical core, an updated version of current FV dynamics, and improved spectral methods which are designed for distributed memory computers. An ambitious, but realistic goal will be to port current and future physical parameterizations to this new core running at the highest resolution.

CAM6 – 2015

Starting with the completion of CAM4, a longer-term roadmap should be developed for the development of CAM. A priority should be the exploration of non-hydrostatic formulations capable of global simulations with a grid spacing of approximately 1 km, which is required to accurately simulate atmospheric convection (Redelsperger and Sommeria, 1986). The difficulty in synchronizing the development of new model dynamics, modifications to the dynamical core and the evolving nature of computer hardware, with the concomitant changes to program models, should not be underestimated. While the development path of CAM5 will be relatively straightforward, the strategy for CAM6 will be less clear and will likely require mid-course corrections at 2-3 year intervals.

b) Future Ocean, Sea Ice, Land, and Land Ice Components

Solutions of ocean climate components in the non-eddy-resolving regime are still more dependent on the quality of the parameterizations used than on the details of the model numerics. However, future development certainly needs to be carried out on both aspects of the model. The recent Climate Project Team (CPT) work on eddy parameterization has resulted in a Gent/McWilliams coefficient that is a function of space and time. Further refinement of the coefficient is desirable and whether the eddies produce a diapycnal component of tracer mixing. It is also important to have an energetically closed formulation of the diapycnal mixing that includes the effects of tides, internal wave breaking, etc. in the deep ocean. The effects of submesoscale eddies is also in the current version, but needs further work which will still be relevant when the ocean component is run at eddy-resolving resolutions of 1/10° or finer. Over the next several years, more and more development work and runs will be done at this resolution, but there will still be the need for non-eddy-resolving versions for very long runs, and applications that need a large ensemble of runs. An early version of an overflow parameterization is also in the present ocean component. This needs to be evaluated and developed further, possibly in conjunction with a bottom boundary layer parameterization. Another possible new direction is to allow for the air-sea interaction to depend on properties of the surface wave field and when they break.

In terms of future model numerics development, the most fundamental would be to move to a model that uses density coordinates in the deep ocean below the strong mixing region. This would reflect the fact that most tracer transport and mixing is along density surfaces in the deep ocean. However, it is still advantageous to keep depth coordinates near the ocean surface. Work in this direction has occurred recently at Los Alamos, with development of a hybrid coordinate version of the POP model, called HYPOP. When this code is fully developed, then it needs to be implemented and evaluated in the coupled framework of the CESM. It should also be compared to the HYCOM ocean model developed by Chassignet and colleagues that also uses hybrid density/depth coordinates which has very recently been implemented in the CESM framework.

Further evaluation of transport schemes that have low dissipation and dispersion needs to continue. The schemes also need to be sign definite when used with the ocean ecosystem model for carbon cycle applications. In addition, fully-implicit time stepping schemes need to be evaluated with emphasis on how to set the necessary preconditioners. If implemented, such a scheme would strongly reduce the computer time needed for long runs, but would it give accurate solutions?

Future versions of the ocean component need to resolve the coastal regions much better than at present. This can be done either by a mesh refinement strategy or by a nested regional model, see Section 6g. There are several reasons for this additional coastal resolution, such as this is where the ocean interacts with the land component, is where much of the ocean's biogeochemistry and biota occur, and where much of the Arctic methane clathrates occur. Potential release of this methane is a very important question and will certainly result in an abrupt climate change if the release occurs with any rapidity at all. Resolving the ocean margins is also important if the CESM is to model the interaction between the ocean and ice shelves in the Arctic and Antarctic. Several small ice shelves have collapsed in the last decade, and the CESM needs to evaluate the potential for the collapse of much larger ice shelves, which could potentially cause a significant jump in the global ocean sea level.

Future development of the CESM sea ice component can also be divided into work on dynamics and numerics, plus work on new parameterizations. The dynamics work includes advances in the sea ice rheology to refine the current elastic-viscous-plastic formulation of Hunke and Dukowicz (2002). The current version of CICE used in CCSM4 is also somewhat sensitive to parameter choices in the ridging and rafting scheme, and further work is needed here, along with refinements to the transport scheme of Lipscomb and Hunke (2004).

In terms of new parameterizations, there are plans to improve the snow physics, sea ice hydrology, and grounded ice. The present snow physics is fairly simple, whereas in reality it is much more complex, with important consequences for both the snow albedo and ice formation as the snow ages. The sea ice hydrology is also very important for the snow albedo, as melt ponds formed during the spring reduce the albedo significantly, which is a positive feedback on the snow melting rate. Experience with the CESM has shown that, if the snow does not completely melt in the Arctic spring, then no surface sea ice melting occurs, and the permanent sea ice becomes much too thick. Sea ice does also play some part in the carbon cycle, and it can be significant in the polar regions where biological productivity is relatively small. In spring, quite large amounts of algae can form on the bottom of the sea ice. In addition, when sea ice melts the dust and iron it contained go into the ocean, which increases the productivity in the polar regions. New parameterizations for these processes are being developed that will be included in further development of the CESM carbon cycle in the future.

All versions of the CCSM to date have required the atmosphere and land components to run on the same horizontal grid. The capability for these two components to run on their own separate grids is presently being implemented, and there are two main reasons for this. The first is that it is anticipated that the atmosphere component will soon move to a non latitude/longitude grid, see Section 6a, whereas the land component will continue to use such a grid, and second this allows the land component to have a fine-mesh capability and use a resolution of 1/10°. This will allow a much better representation of orography and land cover, and result in improved albedo, hydrology, and river transport, for example. These are all important when the CESM will be used to make regional climate predictions for the USA over the next few decades, in order to answer questions such as the future of water resources in the western USA, and permafrost degradation in the Arctic. The increased land component resolution will also benefit the representation of the terrestrial carbon cycle by improved soil and vegetation control of the carbon budget and control of dust emissions by both natural droughts and human induced land cover changes.

New capability over the next several years in the land component will include the following. Close the nitrogen and methane cycles and represent the role of land disturbance on biogeochemical cycling. Further development of the total water cycle will include managed river and lake systems, irrigation, and the river transport of nutrients, chemicals, and sediments. Several human systems will also be included in future versions of the CESM land component. These include agricultural activities, such as crops, animal husbandry, a more sophisticated urban component, human fire systems, and human inputs on soils by use of nitrogen fertilizer, for example.

Observations over the past five years have shown that the Greenland ice sheet is losing mass with more melting than accumulation. In addition, observations in both Greenland and Antarctica show that glaciers have accelerated, especially when small ice shelves at their snouts have disintegrated. These observations have important consequences for future global sea level rise. In response, a small group of scientists, led by Bill Lipscomb of Los Alamos National Laboratory, decided that the CESM needed an ice sheet component. They chose the GLIMMER model developed by Tony Payne at the University of Bristol, see Payne (1999). Over 2008, it has been modified and developed to fit into the CESM framework as a separate component, but very closely tied to the land component. The simplified dynamics of GLIMMER is applicable to the Greenland ice sheet, and so the initial focus is to obtain a good representation of the present day mass balance and ice sheet thickness. Simulations of various paleo epochs will also help define the thermodynamic component of GLIMMER. The focus of this work is to run in 2010 some simulations of the 21st Century that include an active Greenland ice sheet for possible inclusion in the IPCC AR5 report. This will give projections of both the possible sea level rise due to the melting ice, and the effect of the melt water on the strength of the meridional overturning circulation in the North Atlantic Ocean.

In August 2008 a meeting was held at Los Alamos to organize interested scientists from across the USA to further develop the GLIMMER model into a next-generation community ice sheet model, just as the CESM project has done for its physical and carbon cycle components. This development will take a few years, but will produce a component that is able to represent the Antarctic ice sheet, as well as the Greenland ice sheet. The Antarctic ice sheet is more complicated because it has extensive ice shelves that strongly interact with the ocean, in addition to thermodynamic interaction with the atmosphere. This will require the component to include higher-order dynamics which controls glacier flow and variable resolution with unstructured horizontal grids that provide much finer resolution near the ice sheet boundaries. The new component will also require better hydrology parameterizations to represent all the effects of water on the ice sheet. Probably the most difficult aspect is how to model the ice sheet interaction with the ocean that controls how fast the ice sheets melt. This requires much higher resolution in the ocean component that must be provided either by the global model or by interaction with a nested regional ocean component. This is a very difficult problem that will take some time to complete. However, it is important that a future CESM be able to represent the future behavior of the climate system with interactions of both the Greenland and Antarctic ice sheets.

c) Future Biogeochemical and Ecosystem Components

Better understanding of the ecological and biogeochemical feedbacks with climate requires a significant expansion of current CSEM land and ocean model capabilities. Preliminary work in CSM 1 involved the addition of carbon-only land and ocean modules to the physical climate system (Doney et al., 2006); the CSM 1 coupled carbon-climate simulations highlighted many of the issues involved in transient response of the carbon cycle over the 20th and 21st century (Fung et al., 2005). Advances in CCSM 3 included the incorporation of a marine ecosystem model with nitrogen and iron cycling in the ocean. Terrestrial developments included pilot efforts on carbon-nitrogen dynamics, land-cover change, and dynamic vegetation. Ongoing and future work involves coupling of these separate development streams, improving parameterizations of agricultural and urban land, and evaluating model results more rigorously utilizing flux tower, process study and remote sensing data. Implementation of the full scope of nitrogen and phosphorus dynamics and methane and ozone feedbacks requires more sophisticated coupling between land biogenic emissions and atmospheric chemistry. Additional development of land surface parameterizations is also needed, e.g., models of the hydrology and biogeochemistry of wetlands and peatlands.

Land-atmosphere interactions in climate models must be expanded to represent biogeographical processes such as land use, fire, and post-disturbance vegetation succession. A major focus within the CESM project will be the development of the modeling tools and validation datasets for incorporating and assessing historical and future land use; the dynamics of managed forest, rangeland, and agricultural systems; and deliberate land management strategies to mitigate climate change. On an even longer timescale, pilot efforts should begin with integrating natural and social science research with respect to land use, as well as trace gas emissions.

On the atmospheric chemistry side, developmental paths underway will need to be augmented. First, prognostic dust emission, transport, and deposition are being included in the CESM to study both the effects on atmospheric radiation and the impact on ocean biogeochemistry via the dust iron fertilization linkage. Second, reactive chemistry is being incorporated into the model, which is driven to a significant extent by biogeochemical trace gas fluxes from the ocean and land.

Ocean-only experiments have been conducted to assess the effects of atmospheric iron deposition on ocean biological productivity, carbon sequestration, and nitrogen fixation and denitrification. Next steps will involve coupling the atmosphere-land-ocean iron cycle including terrestrial dust production, which is sensitive to vegetation, land-use and water cycle, and more sophisticated iron sources from continental margins. The coastal shelves and continental margins are hot spots of marine biological productivity, fisheries and biogeochemical transformations. Present versions of the CESM do not resolve coastal dynamics well, however, and future improvements will likely depend upon regional nesting within the ocean/atmosphere system.

In the present CESM, the land and ocean biogeochemistry are connected only indirectly via the physical climate, but the land and oceans also interact strongly through the outflow of nutrients and organic matter via rivers and groundwater. Many parts of the world are strongly impacted by coastal eutrophication (high nutrient loading) due to the runoff of excess agricultural fertilizers and sanitation waste, and the problem is expected to grow in the future. Several new modeling activities will be needed to close this land-ocean gap, including runoff of reactive biogeochemical species from the land surface model and downstream transport in rivers; treatment of the biogeochemical transformations that occur in estuaries; high resolution modeling of coupled coastal ocean dynamics; and a dynamic marine sediment-water column module.

d) Future Aerosol and Chemistry Components

The modal aerosol model provides a computationally efficient framework for representing aerosol properties in the CESM, but improvements are needed for several processes. First, to reduce the anthropogenic aerosol indirect effect new sources of natural aerosol need to be added, including primary and secondary marine organic aerosol. Second, emissions of mineral dust need to be speciated to distinguish between components with different optical properties, different microphysical properties, and nutrients important for fertilizing ocean biology. Third, the size distributions of emissions of primary particles, particularly those arising from combustion, needs to be constrained better with field measurements. Fourth, emerging advances in the treatment of new particle formation should be implemented. Fifth, new understanding and proposed mechanisms of formation of secondary organic aerosol should be applied. Sixth, recent more accurate and computationally efficient treatments of aerosol thermodynamics and water uptake should be considered. Seventh, effects of aerosol on shallow cumulus clouds should be added to the shallow cumulus scheme, and new treatments of the effects of aerosol on ice clouds should be considered. Finally, an alternate method of representing the aerosol moments should be introduced.

One interesting and challenging topic for Earth System Models is the possibility of fully coupling atmospheric chemistry with the global biogeochemical cycles of key species. This coupling would include coupling of the i) the nitrogen cycle; ii) the carbon cycle; iii) the sulfur cycle and iv) the chlorine and bromine cycles between the land, ocean and atmosphere. The complex nitrogen cascade which occurs after the introduction of reactive nitrogen into the environment involves not only many species, but the interaction of all components of the earth's surface (snow, land, water) with the atmosphere. The increase of environmental reactive nitrogen over the 20th century is largely linked to agriculture. However, the critical nitrogen transformations that occur locally within the soil are communicated to the atmosphere where they play a critical role in regulating the concentration of greenhouse gases including nitrous oxide and ozone. The terrestrial carbon cycle is impacted by atmospheric nitrogen deposition and ozone. It is directly linked to the atmosphere through the emission of methane and biogenic species. The resulting emissions are sensitive to climate change through changes in wetland distribution and changes in temperature and CO_2. In turn, they impact climate by regulating the concentration of the greenhouse gas methane as well as atmospheric aerosols. Likewise sulfur (as DMS) and chlorine and bromine (as halogens) emissions from the ocean are an additional link between atmospheric chemistry, climate and global biogeochemical cycles.

Additional challenges include an improved representation of the dynamical and chemical coupling between the stratosphere and the troposphere in Earth System Models, as well as an improved representation of megacities. Urban emissions are expected to change significantly over the next century due to an increased number of megacities, especially in the tropical regions. While models are significantly improving in their horizontal resolution, we envision developing a representation of chemistry within the Community Land Model such that the nonlinearities in the chemistry can be represented at the size of the CLM grid, then distributed to the atmosphere. This would enable a much improved representation of urban chemistry, and its impact on the large-scale chemistry and climate. An important aspect of this would be improved representations of the interactions between gas-phase chemistry and aerosols whose representation is currently either simplified or not included in the CESM. Examples include the production of secondary organic aerosol precursors, sulfate, nitrate, and ammonia by chemistry, and the effect of aerosols on photolysis and heterogeneous surface reactions.

e) Future WACCM Component

Long-term development of WACCM will lead to advances in both the dynamical and physical components of the model. The way WACCM parameterizes gravity waves will be improved in two areas: momentum conservation at the source and top of the model; and the thermal effects of dissipating waves (diffusion, thermalization of wave energy) will be re-evaluated and refined by comparison with observations. Modifications will be carried out with the goal of internally generating a quasi-biennial oscillation (QBO) within WACCM. Necessary changes will likely include the following: (a) fine (sub-kilometer) vertical resolution; (b) highly scale-selective hyperdiffusion; and (c) a convective heating parameterization that produces large variability at time scales from 10 days to a day or less.

Now that CAM-CHEM and WACCM utilize the same code base, the chemical solver and method of specifying a chemical reaction scheme are identical between the models. Further chemistry package development is planned with the goal of unifying the chemical codes across CAM-CHEM/WACCM and WRF-CHEM. It is also planned to unify photolysis and heating calculations within these models; currently these are independent calculations. For particulate and cloud studies in the lower, middle and upper atmosphere, a sectional microphysical model (CARMA) will be incorporated into WACCM. Simulations using this model will aid in further development of microphysical parameterizations in WACCM.

Development plans for WACCM-X (a version with model top at ~500 km) include development of modules that resolve ion and electron transport, ambipolar diffusion, and include an ionospheric dynamo. Modification of the dynamical core will be necessary to simulate horizontal molecular diffusion and ion transport. There are also plans to couple WACCM-X with a plasmasphere model (the Global Ionosphere and Plasmasphere), and a magnetosphere model (the Lyons-Fedder-Mobarry model).

f) Future Paleoclimate Developments

The success of a vibrant paleoclimate program within the CESM depends on achievement of the following developments:

The development and maintenance of a low-resolution version of CESM. The paleo record demonstrates rapid and dramatic changes in ocean circulation and climate on timescales from decades to tens of thousands of years. To understand the mechanisms that determined the state of the past Earth requires the capability of running a matrix of simulations with CESM for thousands to tens of thousands of years. The attribution of natural variability and forcings in defining past climate sensitivity requires a systematic experimental design that can only be accomplished with a hierarchy of models of varying complexity. It is essential that the CESM project retain as a high priority the development and maintenance of low-resolution versions of the CESM.

The incorporation of paleotracers within CESM. Past climate changes are recorded in ice cores and ocean sediments using tracers that are not currently simulated within the component models of CESM. In order to gain an understanding of whether the CESM is able to replicate such changes, it is essential to be able to simulate the tracers that are recorded in the observational record. The first paleotracers to be incorporated into the model should be $\delta^{18}O$ (used for assessing atmospheric temperature, precipitation, and ice-volume changes from water isotopes in polar and tropical ice cores); radiocarbon (which yields information on changes in rates of ocean ventilation); and $\delta^{13}C$ (which has been widely used to infer dramatic shifts and re-organizations in ocean circulation).

Development of the capability for CESM to simulate past ice sheets. The GLIMMER and CISM ice sheet models currently being developed by the new land ice working group concentrate on the stability of the Greenland and Antarctic Ice Sheets. Understanding the dynamics of past climates requires the development of a framework that includes other land-based ice sheets, and incorporates the response of the bed to changing ice load of isostatic rebound.

Further development of the marine and terrestrial biogeochemistry in CESM. The quantitative and mechanistic explanation of atmospheric carbon dioxide variations over the glacial-interglacial cycles of the last million years remains one of the major unsolved questions in climate research. Simplified models suggest that no single mechanism can be invoked, but rather that physical and biogeochemistry changes in the ocean and over land need to be considered and that the relative importance varies as the climate state changes. To fully assess the processes responsible for past variations will require inclusion of new features to the biogeochemistry modules, for example, coral reef regrowth and an ocean sediment model.

Development of a framework to model atmospheric chemical state of past Earth. Atmospheric chemistry simulations for the latest Permian indicated that release of H_2S led to an increased methane lifetime, which would have caused a collapse of the ozone layer. Hydrogen sulfide in high concentrations is directly toxic to many life forms. A frontier for CESM is to investigate the interaction of physical and chemical processes for the habitability of Earth.

g) Nested Regional Climate Models

The climate research community is beginning to use higher resolution (~50 km) models for the decadal prediction problem, but global modeling frameworks that resolve mesoscale processes are needed to improve our understanding of the multi-scale interactions in the coupled system, identify those of greatest importance, and document their effects on climate. Ultimately, such basic research will help determine how to better represent small-scale processes in relatively coarse resolution Earth System Models (ESMs). The impact of small-scale processes on larger scales is often termed "upscaling".

There is a wide range of upscale interactions to be considered. Current parameterization schemes do not adequately handle the mesoscale organization of convection, which is a critical missing link in the scale interaction process. The limited representation of convection and cloud processes is likely a major factor in the inadequate simulation of tropical oscillations. Cloud and convective processes also appear to play a role in the well known double Inter-Tropical Convergence Zone (ITCZ) bias issue, though coupled processes involving a systematically intense equatorial cold tongue in the ocean also likely contribute to this persistent systematic error in many coupled models.

Uncertainty in the representation of clouds (on all scales) is also a major influence in the response of the climate system to changes in radiative forcing. Improved simulation of cloud processes in the Multi-scale Modeling Framework (MMF), which embeds two-dimensional cloud resolving physics within three-dimensional weather scale physics, has shown improved MJO variability and reduced the bias in Kelvin wave propagation.

Another scale interaction problem is the challenge in modeling the Subtropical Eastern Boundary (STEB) regimes off the coasts of Southwest Africa, Peru-Ecuador-Chile, and Baja-Southern California. These regimes are marked by marine stratus, equatorward alongshore winds, and ocean upwelling. Large and Danabasoglu (2006) suggest that better resolution of these features produce not only a better simulation of the regional climate, but also effects that propagate and strongly influence the large-scale climate system, reducing rainfall biases across the tropical oceans.

Other examples of “hot spots” with significant upscaled effects include the monsoon regions of India and Tibet and Central and South America where steep topographical gradients and mesoscale processes such as low-level jets and mesoscale convective complexes play an important role in the water and energy budgets locally and remotely. Over the Maritime Continent, Lorenz and Jacob (2005) presented a study of two-way coupling using global and regional models, and demonstrated large and positive impacts on the tropospheric temperature and large scale circulation in the global climate simulation.

Clearly, addressing these errors is critical to climate prediction on all time scales. Therefore, there is a strong need to develop pilot projects to demonstrate the methodologies and impacts of multi-scale interactions on the regional and global climate. While numerical models and techniques will be central to this effort, so too will be sophisticated theoretical and physical research to both understand and specify the critical interactions.

One pilot project that has been developed is the “Prediction Across Scales” initiative at NCAR. This initiative is a collaborative effort between CGD, MMM and interested participants from the broader (CCSM and WRF) community to coordinate research and system development activities across weather and climate scales. Recent major advances in petascale computing, coupled with rapid advances in scientific understanding, are enabling progress in simulating a wide range of physical and dynamical phenomena with associated physical, biological and chemical feedbacks that collectively cross the traditional weather-climate divide. Such simulations and predictions are essential to a society that is becoming much more sophisticated in its requirements for weather, air quality and climate predictions and that is able to make useful economic and social use of such improvements. Moreover, as discussed above, fundamental barriers to advancing such prediction on time scales from days to years, as well as long-standing systematic errors in weather and climate models, are partly attributable to our limited understanding and capability to simulate the complex, multiscale interactions intrinsic to atmospheric and oceanic fluid motions.

The enabling tool for this type of research will be the Nested Regional Climate Model (NRCM). The result of this ambitious effort to combine high resolution regional atmosphere and ocean models with a state-of-the-science climate model will be fundamental progress on the understanding and prediction of regional climate variability and change. In particular, embedding the WRF and a Regional Ocean Model System (ROMS) within CESM will allow scientists to resolve processes that occur at the regional scale, as well as the influence of those processes on the large-scale climate, thereby improving the fidelity of climate change simulations and their utility for local and regional planning. More information on NRCM, including existing and planned numerical experiments, can be found at www.nrcm.ucar.edu

h) Algorithms and Computational Environment

Future generations of Earth System Models will face significant algorithmic and computational challenges. The present petascale computers consist of hundreds of thousands processing elements with a complex memory hierarchy. We expect that the next generation exascale machines will have factors of 100s more processing elements requiring millions of parallel threads of execution. Computer chip manufacturers have abandoned the increase in clock rates and now rely on adding ever more cores to improve performance, challenging application programmers to identify finer grain parallelism and manage deeper memory hierarchies for efficient computation. Since these platforms may arrive as early as 2015, new approaches and paradigms will need rapid development in order to take advantage of the science opportunity presented by this computational power.

Scalability will be a critical requirement of every component in the next generation Earth System Model. The biggest scalability bottleneck in today's Earth System Models is the atmospheric dynamical core. This bottleneck is created by the pole problem introduced by the use of latitude/longitude grids. New dynamical cores with cubed sphere and icosahedral grids, along with yin-yang (baseball) and other overlapping systems, show promise for scalability in highly resolved models. In addition, new coupling mathematics algorithms will also be required. To develop the ability to predict future sea level rise, ocean circulation and to understand the effects of climate change on extreme events, new components will be added to the model. New physics and many new scales will also be introduced, and thus require research into the best multi-physics and multi-scale coupling strategies. The human dimensions of climate change will also begin to be more closely integrated with the physical models for sustainability studies and consistency with decision support and integrated assessment modeling. All new techniques will need to be developed from inception with *scalability* as a key requirement. In addition, the time it takes for model developers to incorporate and evaluate new components will need to be dramatically reduced, thereby also requiring the need for research into improved verification and validation strategies and an investment in associated software engineering support.

Another critical computational challenge for the next Earth System Model will be to determine the optimal programming model for the anticipated new computing architectures. The requirement that models run efficiently on processors with many more cores than they have today, but with little increase in the processor's memory bandwidth, jeopardizes current programming practices. In the current petascale environment where the number of cores per socket is relatively small, we expect that the hybrid MPI and OpenMP paradigm will be adequate (Drake, et al. 2008). However, as we move towards scenarios where we expect applications to run on systems with millions of cores and diverse architectures, it is doubtful that this will continue to be the case. These new architectures will need to be programmed with techniques exposing finer grain parallelism and where computation is coordinated with the memory hierarchy. Scalability and reproducibility will also be key requirements. The current programming models (MPI+Fortran) and fault tolerance approaches are not scalable, and the likelihood of undetectable errors will increase without new improvements to fault detection and better resilience strategies. In addition, computer vendors are also considering embedded processor technology that could permit multiple systems to be built, each specialized to a particular class of problems in order to address the cost and power barriers faced by conventional approaches. If these approaches can be successfully applied to resolving climate modeling computational bottlenecks, then the climate science community will face even greater programming challenges. Finally, fault resilience and auto-tuning will be needed in order to enable better throughput and efficient utilization of hardware resources. Such a new programming infrastructure is required in order to enable sustained performance on upcoming systems. Without this, we may fail to meet the performance requirements necessary to achieve the desired science impacts. Since there are many options for programming models in the 5-10 year time frame, and code conversion would take nearly as long, an experimental approach to prototype parts of the model should be pursued.

Practical simulations for decadal prediction and ensemble runs will also require revisiting the software architecture and ensuring effective parallel I/O that achieve rates of 100's of GBs. Due to the many requirements on the I/O subsystems of these models, a more flexible utility structure is needed that is supported and available across centers and hardware and software vendors. This issue will only be aggravated by the use of unstructured grids or by the selective output of extreme events. Improving I/O performance will also be necessary in order to support the dramatic increase in data generated by ensembles of long time simulations required for studying extreme events and by those needed for decadal predictability efforts. The shortest term goal within the next 5 years is to develop new parallel I/O systems at all levels.

As Earth System Models become increasingly complex and high performance computing architectures change faster than ever, CESM will need to work with the modeling community to develop programming models and auto-tuning technologies (as a risk mitigation strategy) for the next generation Earth System Model that offer performance portability and fault resilience. A concerted effort to prototype key climate algorithms to understand the relative merits of alternative programming technologies will need to be a high priority. Obtaining reasonable performance on multi-core platforms will require better performance introspection to do auto-tuning, and a better understanding of causality with sufficient coverage by instrumentation, to understand performance. A programming model is necessary, but not sufficient. Scaling to millions of processing cores will also require parallel scalability in *every* aspect of the climate model. The end result of both of these efforts will be to enable simulations with the most complex Earth System Models that will effectively utilize exascale class systems.

7) Resources Needed to Accomplish the CESM Goals

Resource needs can be divided into two categories: people and computer resources. Resources for scientists and software engineers have diminished over the years 2004-2008. The consequent reduction in people working on the project meant that progress has been slowed down. New knowledge and developments have not been incorporated into the model rapidly enough. There were too few people to modify and run the models for development, scientific exploration, and assessment-type production runs. This led to a rationing of resources determined by program priorities. IPCC-type runs, done as part of the CCSP commitment to the IPCC assessments, while a critical part of the process and method of model evaluation, have nonetheless come at the expense of model development and research. This science plan calls for strongly enhancing the human resources needed to avoid this rationing in the future. Better links between the process research and parameterization programs are needed in order to move their developments more rapidly into the core model. Further, if the enhancement is large enough, it will be used to connect with the consumers of simulation output, such as the Integrated Assessment and

Ecological Impacts communities, to give them much easier access to CESM data. However, the envisioned enhancement requires a substantial investment in both scientists and software engineers to make the strong connections between the process research, the models and users of climate model output. This will allow NCAR, DOE laboratories and University collaborators to leverage the investments in computational science and information technologies made by the DOE Office of Science and the NSF across all the fields of science it supports. As this plan was being finalized in early 2009, there are hopeful signs that the budget of the CESM project will have a reasonable increase in FY10.

The second category is computing resources, which, in contrast to human resources, have increased significantly over the past five years. This has enabled the CCSM project to contribute to the AR 4, and subsequently develop the CCSM 4. However, frequently testing and development of the next generation of model components are delayed to meet the near term production needs for future scenario projections. This "either/or" situation is not healthy. Climate modelers need a range of resources, from desktop to leadership-class computing capabilities, data management and archive centers and the people to manage them. The CESM project requires dedicated, large capacity resources from the DOE leadership-class centers at several of their laboratories, the Climate Simulation Laboratory run by NCAR, and, in addition, the NSF Tier I computational centers, with appropriate human and data storage support around them to optimize their benefit for climate modeling.

8) Products

An Earth System Model framework that can be used for basic science research, future climate projections, and decadal forecasts. Model versions will be formally released when appropriate, which is at least every few years and probably timed to synchronize with the IPCC assessment report schedule. Model code that is freely available from the CESM web site, and free access to the output from the suite of runs performed for IPCC reports.

A system of working groups that allows any interested scientist to become involved in the project, so that ideas can be evaluated and incorporated into the model. Meetings of these working groups and the annual workshop are forums where students can be trained in the science of climate modeling and analysis of the model output and observations.

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APPENDIX 4: UQ METHODOLOGY

DESCRIPTIONS OF CROSS-CUTTING UNCERTAINTY QUANTIFICATION METHODOLOGIES

This appendix provides more detail about the uncertainty quantification (UQ) methods discussed in Chapter VI. These methods include sensitivity analysis, construction of surrogate response surfaces, input parameter calibration, forward uncertainty propagation, and model uncertainty quantification. Although these UQ methods have been tested in multiple applications involving complicated models of physical phenomena, they may require modification to customize and apply them to CSSEF models and observations. The overall goal with each of the component sections (atmosphere, ocean, and land) will be to characterize uncertainty in model parameter values; assess the sensitivity of predicted response uncertainty associated with input parameter uncertainty; calibrate the input parameters of the model (often with multiple, heterogeneous data sets); assess structural (model discrepancy) uncertainty; and, propagate these multiple uncertainty components forward to generate an overall estimate of prediction uncertainty. We envision this as an iterative process that will be repeated as new observational data sets and new process model (structural and parametric) understanding is brought to bear.

SENSITIVITY ANALYSIS

Sensitivity analysis (SA) methods enable means of identifying "influential" uncertain input variables. This information is useful for enhanced understanding of model response. It is also important for down-selecting important variables, thereby reducing the requisite dimensionality of the input space for UQ studies and surrogate response surfaces (emulators). We focus on global SA methods, and we expect global approaches to complement local SA methods. There are a variety of global SA approaches that can be used (Saltelli et al. 2001). These include graphical and statistical analysis methods, variance-based decomposition (VBD) for attribution output variability to inputs, and Morris One-At-a-Time (MOAT) for main effect analysis. Currently, most SA methods are available in common open-source statistical analysis and UQ packages, such as R and the Design Analysis Kit for Optimization (DAKOTA).

We will use SA methods, such as MOAT, to provide information on important parameters, thereby enabling a priori reduction of the dimensionality of the input space and allowing for feasible means of construction of surrogate response surfaces for subsequent UQ studies. On the other hand, many SA methods are computationally expensive on high-dimensional problems, especially the calculation of the global sensitivity indices in VBD. These methods would typically be used a posteriori, employing an emulator already built over the input space using an ensemble of simulations (e.g., Storlie et al. 2009). Sudret (2008) and Tang (2010) derived the VBD indices based on polynomial chaos expansions (PCEs) and stochastic collocation, respectively. The advantage of these approaches is that the VBD sensitivity indices are analytic expressions of the expansion coefficients and thus one obtains the sensitivity analysis "for free" once the expansion is created. Similarly, Oakley and O'Hagan (2004) and Gramacy and Lee (2008) used Gaussian process-based emulators in a Bayesian framework to estimate VBD sensitivity indices, including producing error bars on the resulting indices (due to imperfect surrogate models). Both emulator and PCE-based VBD indices have been shown to be as accurate as Latin Hypercube Sampling (LHS)-based VBD indices using three-orders of magnitude fewer function evaluations (Weirs et al. 2010).

A promising efficient (local) SA for components or specific processes of the climate models is the use of automatic differentiation (AD), which is an intrusive approach to SA. It offers the capability of efficient computation of local sensitivity information.

STATISTICAL RESPONSE SURFACES

The quantities of interest (QOIs) from climate simulations will include spatiotemporal summary statistics across multiple output variables. Given the computational expense of a single climate model simulation at a fixed set of input parameters (IPs), there is clear value in building accurate surrogate models (also called meta-models, emulators, or statistical response models) that represent IP-to-QOI dependence. Such surrogates can then be queried extensively for both forward and inverse UQ, detailed sensitivity analysis, or for optimization purposes. As the surrogate model is just an approximation to the IP-to-QOI relationship, uncertainty in the estimation of the surrogate has to be accounted for in the downstream UQ analysis. The goal is to develop and explore multiple types of surrogate models for added robustness in the UQ analysis relying on surrogate models.

Spline-based Surrogate Models. Multivariate Adaptive Regression Splines (MARS) (Freidman 1991) model the response using a sum of tensor products of spline basis functions with local support. The basis functions are selected using a forward stepwise procedure to add terms followed by a backward pruning process that strives at balancing fidelity to the response data and model complexity. MARS is a nonparametric surface fitting method that is not constrained by passing through all of the response data values. Thus, it provides some smoothing of the data. There currently exist multiple (open source) implementations of various variants of MARS.

Polynomial Chaos Expansions. PCEs (Ghanem and Spanos 1991) provide an efficient, flexible framework for surrogate model construction. PCEs employ orthogonal polynomial representations of a QOI over the IP space. They can be employed as global, or local element-based, functional representations. They can be constructed using nonintrusive sampling methods, where the samples are used to provide numerical estimates of projection-integrals for the PCE coefficients. Both random (Monte Carlo and various variants), and deterministic (quadrature/sparse-quadrature) sampling methods for PCE construction are available in DAKOTA. When, after reduction of IP space dimensionality, the requisite number of random or deterministic samples is still not computationally feasible, we will use Bayesian methods for PCE surrogate estimation, employing Gaussian Process (GP) models.

Gaussian Process Models. Broadly, GP emulators provide another class of surrogate surfaces. Since there is uncertainty associated with the lack of knowledge of the climate model output at nonsampled IP values, GP interpolations (aka “kriging” predictors) provide probabilistic assessment of the state of knowledge of a QOI for IP values at which the forward model has not been evaluated (Sacks et al. 1989; O’Hagan et al. 1999; Rasmussen and Williams 2006; Santner et al. 2003). Sparse GP approximations using maximum likelihood (e.g., Sacks et al. 1989) or Bayesian methods (e.g., Gramacy and Lee 2008) are typically required to tackle the computational cost of training GP surrogates (Snelson and Ghahramani 2006).

High-dimensional Response. To circumvent the computational expense of sampling high-dimensional GPs and to obtain a reduced-order model for the process, we will also employ Karhunen-Loeve (KL) expansions (Karhunen 1946, Loeve 1955) that represent a stochastic process as a linear combination of a countable number of uncorrelated random variables (Higdon et al. 2008). Where needed, we will couple GPs with PCEs, either by having the GP mean trend as a PCE, or by obtaining uncertain PC coefficients via orthogonal projection of the GP sample surfaces (viz. Bayes-Hermite quadrature, see O’Hagan 1991).

Adaptive Sampling. One ultimate goal is to use as few climate simulations as possible to train an emulator to achieve the needed predictive accuracy. We will pursue adaptive sampling methods for maximal efficiency, driven by an improvement criterion that aims at maximizing predictive accuracy, either locally or globally. In the GP context, this criterion can be based on the variance of the GP prediction at the given IP value, as for example in Gramacy and Lee (2009) and Gramacy and Polson (2010).

INPUT CALIBRATION METHODS

Calibration of input parameters, also called parameter estimation or the inverse problem, refers to determining optimal parameter settings for a model so that agreement is maximized between model calculations and a set of experimental data. There are two main classes of methods: optimization methods, which use regression to characterize parameters based on minimizing a sum-of-squares error term using optimization, and Bayesian methods, which rely on Bayesian inference to construct joint probability density functions (PDFs) over multiple parameters which are consistent with the data and with the assumed form of the likelihood function.

Optimization (Nonlinear Least Squares) Methods

Often the criteria for calibration is to minimize the sum of the squared residuals (where residual is the difference between the model prediction and the experimental data) (Seber and Wild 2003). This is typically called minimizing the “sum squared error.” There are more sophisticated objective functions based on information theory, such as Akaike’s information criterion which seeks to balance model complexity with model precision. In general, optimization uses an iterative method (examples include quasi-Newton and projected conjugate gradient) to fit an objective function, using local calculations of first-order and sometimes second-order local parameter space gradient information.

The optimization approach depends on evaluation of local gradients (first and sometimes second order) in multidimensional parameter space. Given gradient information, the iterative optimization methods can be very rapidly convergent, requiring far fewer forward model evaluations than Bayesian methods. While finite difference approximations of gradients are possible, the number of required forward model integrations is proportional to the number of gradient elements, and the results suffer from round-off and approximation errors. A different approach uses automatic differentiation (AD) to generate gradient information. AD generates augmented model code which introduces new variables and calculations in all the original model algorithms to provide gradient information through application of the chain rule for partial differentiation of a complex function. AD can be applied either in forward mode (linear tangent method) or reverse mode (adjoint method), differing in the order in which the complex partial derivatives are calculated.

Forward mode AD is most computationally efficient when the number of input parameters is small but the number of outputs is large–such as in the case of optimizing a few parameters against individual records from a long time series of surface carbon, water, and energy flux observations. Reverse mode AD is most efficient for a large number of input parameters and a small number of observables, for example when optimizing many gridded carbon state variables against aggregated regional-scale productivity or biomass observations. Automatic code generation tools are available for both forward and reverse AD, but the forward AD tools are considered more tractable for complex models such as the Community Land Model (CLM). The work proposed in this document will investigate forward AD, but will explore the use of model adjoints (reverse AD) as we gain both experience with the application of these methods and operational knowledge of the model sensitivities and available observations. For either forward or reverse AD, estimation of parameter and prediction uncertainty will require that we adopt an explicit error model, taking care to account for time series correlation in the case of multi-temporal observables.

BAYESIAN INFERENCE APPROACHES

The assessment of uncertainties in climate model inputs can be reduced to the estimation of posterior distributions, conditioned on available data, of model parameters and field variables. The latter are used to represent uncertain functions (e.g., boundary conditions), model structural errors (shortcomings of a model due to missing/inaccurate physics) and handle the “missing data” problem in derived data products. Parameter estimation activities on component models (e.g., CAM) will be performed with their surrogates and using, for example, Markov chain Monte Carlo (MCMC) techniques for posterior inference may suffice. We will also allow models of modest/tractable computational expense, such as column models in CLM, to be used “as-is” (i.e., without recourse to surrogates) in parameter estimation by incorporating scalable posterior sampling algorithms (such as multi-chain MCMC). Below we describe proposed calibration-related methods and the adaptations required for use with the CSSEF’s models.

Low-dimensional random field models. Gaussian process models, along with Bayesian model fitting techniques, are routinely used to represent smooth, stationary fields in the Earth sciences (e.g., Mueller et al. 2008). In conjunction with their truncated KL expansion, they also form a low-dimensional model. They are very useful when the field being estimated is related to the observables by a process/PDE-based forward problem (Marzouk et al. 2007). Random field models sometimes requires the use of “sparsifying” priors (Romberg et al. 2001; Vaswani 2010) in case dimension reduction via KL expansions are not easily tenable (e.g., in case of multiscale models). Efficient priors are generally specific to the problem at hand and will be developed in the proposed research effort.

Scalable adaptive posterior sampling techniques for parameter estimation. MCMC techniques, in conjunction with field models, have been successfully demonstrated on watershed and subsurface flow problems (e.g., Ray et al. 2009) and in climate related applications (e.g., Wikle et al. 2001) for posterior inference. However, most MCMC techniques are serial and cannot be used with computationally intensive models without recourse to surrogates. Multi-chain sampling techniques (e.g., Shuffled Complex Evolution Metropolis (Vrugt et al. 2003) and Differerential Evolution Adaptive Metropolis (Vrugt et al. 2009) have been demonstrated in inverse problems using PDE-based simulators (Vrugt et al. 2008). Such techniques have been combined with Ensemble Kalman Filters (EnKFs) to perform joint estimation of time-dependent states along with time-independent model parameters (Vrugt et al. 2005), and have shown to scale well in some cases (e.g., Peters et al. 2004). In contrast, deterministic parameter estimation methods (Tarantola 2005, Adams et al. 2010) have been demonstrated on extremely large problems (Akçelik et al. 2005) and their scalability and robustness are not in doubt. Another promising family of scalable algorithms for posterior inference is based on population and sequential Monte Carlo (PMC and SMC) samplers (e.g., Doucet et al. 2002).These were originally developed for dynamic systems, but have been adapted to static inference problems (Moral et al. 2006; Jasra et al. 2007). SMC scales very well as large number of posterior realizations (“particles”) are evolved simultaneously. Johannesson (2009) demonstrated the use of SMC for Bayesian parameter inference, using GP-based surrogate model trained with adaptive sampling of the forward model and driven by efficient posterior inference of unknown input parameters.

Note that we anticipate some development needed for Bayesian calibration applied to climate applications. This includes developing a library of spatial random field models, with emphasis on integration with sampling and filtering techniques. Of particular interest will be the development of efficient (“sparsifying”) priors of relevance to climate science/process models. Parameter estimation libraries, containing both serial and parallel MCMC, EnKF, and SMC-based algorithms, will be developed for use with climate-related data and models.

Structural Error. The characterization and estimation of any potential structural model error is an integral part of calibration. In line with (Kennedy and O’Hagan 2001), we will use a (sparse) random field representation for the structural error of a climate or process model and assume its independence from both the model’s predictions and its calibration parameters (e.g., Higdon et al. 2008). In this framework, structural error and uncertain input parameters are estimated simultaneously. Bayesian model averaging concepts will be explored to calibrate model ensembles (to training data) in an effort to reduce the impact of the structural error of individual models (Raftery et al. 2005).

FORWARD PROPAGATION OF UNCERTAINTY

Forward UQ refers to propagating uncertainties in the model inputs, such as initial and boundary conditions and model parameters, through the simulation model in order to assess the effect of those uncertainties on the model predictions. Our main focus will be on the use of nonintrusive, sampling-based approaches for forward UQ. Two classes of sampling methods will be used: random and deterministic sampling.

Random sampling methods. These methods generate samples from input distributions, run the simulation at the sample points, and then analyze the resulting distributions on the outputs. Random sampling methods include Monte-Carlo, a number of flavors of Quasi-Monte Carlo sampling, such as LHS and importance sampling, as well as Centroidal Voronoi Tesselations, and classical experimental designs. Most sampling methods are not adaptive. However, climate applications will require adaptive sampling, and we plan to use two approaches: (1) an approach which “augments” an LHS sample by doubling it with a set of points that maintains the stratification and correlation of the original sample and (2) importance sampling, which selectively samples “important” values of input variables to improve the estimation of a statistical response quantity. Importance sampling can be challenging to implement efficiently. Swiler and West (2010) examined the use of kernel density estimators in an adaptive importance-sampling context, which could be tailored to climate simulations. Similarly, Gramacy and Lee (2008) explored adaptive sampling methods driven by the predictive accuracy of a GP surrogate model. Broadly, Monte Carlo/Quasi Monte Carlo methods are attractive in that they are not/mildly sensitive to dimensionality, in contrast with deterministic sampling. Moreover, random sampling methods do not rely on any smoothness of the system response. With respect to analyzing climate model uncertainties, we note that there are many regulatory precedents for using random sampling methods for large-scale risk analyses of high-consequence events such as nuclear waste repository performance (SNL 2008) and nuclear power safety (USNRC 1975).

Deterministic sampling methods. Deterministic sampling methods are commonly used in non-intrusive PC UQ methods for quadrature/sparse-quadrature (Q/SQ) evaluation of projection integrals for PCE coefficients. In this context, forward-model simulations are evaluated at parameter values chosen at the Q/SQ points. While these integrals can be also evaluated using random sampling, Q/SQ methods are more efficient than MC/LHS for small to moderate dimensionality. By taking advantage of known/presumed smoothness in the QOI, these deterministic sampling methods can achieve fast convergence with generally fewer samples than Monte Carlo/Quasi Monte Carlo methods (Eldred and Burkardt 2009, Eldred et al. 2008, Eldred and Swiler 2009).

Whether employing random or deterministic sampling, the resulting PCE for the QOIQOI is an efficient and flexible polynomial surrogate for the forward model. Frequently, however, smoothness properties are not satisfactory, and QOI dependence on inputs can be strongly nonlinear or discontinuous. This can in principle be addressed using local PC and domain decomposition approaches (LeMaitre et al. 2004, Sargsyan et al. 2009, Sargsyan et al. 2010, Wan and Karniadakis 2005). However, this approach does not scale well with dimensionality. We will enhance these techniques by identifying discontinuity locations in the forward models via Bayesian inference, and using parsimonious domain decomposition with large partitions of input parameter space where the QOI is sufficiently smooth (Sargsyan et al. 2009). Moreover, PC expansions typically minimize an error measure that weights against low-probability regions of input space. This can lead to surrogate models that are not accurate enough in PDF “tail” regions. To mitigate this, we will employ PCEs with heavy-tailed standard RV bases (e.g., lognormal), as well as customized polynomials that are orthogonal with respect to probability densities of input parameters (Gautschi 1982).

The main challenge with deterministic sampling PC UQ methods is the strong sensitivity to dimensionality of the input space. Approaches to mitigate this curse of dimensionality include various variants of adaptive anisotropic sparse quadrature (SQ) methods, where important dimensions are sampled more extensively. These approaches are currently implemented in the DAKOTA toolkit (Adams et al. 2010), and can be made available/coupled to the climate toolkit framework. However, these techniques are computationally feasible up to moderate—say ten to twenty—dimensions, depending on the CPU cost of one model evaluation. Even after sensitivity analysis and down-selection of influential parameters, climate model or testbed input parameter spaces can exceed this regime. Beside the Bayesian PCE/GP approach discussed above for resolution of this challenge, one can employ reduced order approximations to capture the most relevant dimensions or manifolds in the input space. For example, High Dimensional Model Representation (HDMR) effectively decomposes smooth functions of multiple parameters into sums of simpler, lower-dimensional functions. It takes advantage of the inherent property of many physical models that the system behavior is dominated by independent individual contributions from parameters (Rabitz and Alis 1999; Ma and Zabaras 2010). The Proper Generalized Decomposition is another approach that approximates a high-dimensional function in terms of a combination of low-rank components (Nouy 2007), while kernel based methods, e.g., diffusion maps or geodesic maps, discover nonlinear dependent structures and effectively reduce the dimensionality of the input space (Coifman and Lafon 2006; Ganapathysubramanian and Zabaras 2008).

The development and adaption of forward UQ methods will be driven by the needs of the UQ tasks in the components.

MODEL UQ

Model UQ includes quantification of structural error (also called model discrepancy: the difference between data and the model) and model uncertainty (also referred to as "model plausibility," the likelihood of a given model based on the available data). We will use Bayesian methods for model UQ. This includes methods for model comparison, selection, averaging, and validation. We will also use "fingerprinting", as further outlined below.

Model Comparison. We will develop Bayesian model comparison methods employing model "plausibility". This methodology favors model parsimony and avoids overfitting. It has a built-in quantitative implementation of the Ockham's razor principle, penalizing models that are too complex, and that learn too much from the data (Beck and Yuen 2004). Given a set of candidate models of interest $M=\{M_1, M_2, \ldots\}$ where each model M_i is characterized by its uncertain parameter vector λ_i, model plausibility is defined as the marginal posterior probability of the model conditioned on data, $p(M_i|d)$. This probability is evaluated from Bayes theorem: $p(M_i|d)=p(d|M_i)p(M_i)/p(d)$, with $p(d)=\Sigma_i\, p(d|M_i)p(M_i)$, and where $p(d|M_i)$ is the marginal likelihood for M_i, and $p(M_i)$ is the prior probability for M_i. Likelihood functions, involving model computations of particular observables, will be evaluated using surrogates in order for these methods to be practical.

Model Selection. We will use Bayesian model comparison, employing model plausibility for model selection, when one model has overwhelming plausibility. With identical priors on models, this amounts to identifying the model with the largest marginal likelihood, or the largest Bayes Factor. Depending on the number of uncertain parameters, and the computational cost in evaluating Bayes factors, we will rely on approximations, e.g., AIC, BIC, or Laplace's method (Kass and Raftery 1995).

Model Averaging. We will employ Bayesian Model Averaging (BMA) for prediction of a QOIQOI with uncertainties reflecting the marginal prediction of the set of plausible models, when there is not one model with overwhelming plausibility. Employing BMA, the prediction of a given QOI is evaluated based on $p(y|d)=\Sigma_i\, p(y|M_i,d)\, p(M_i|d)$, where measures of the plausibility of the models provide weighting for posterior predictions of each model. This requires specifying a set of plausible models, which can be a challenge depending on the situation at hand. Further, dependences among alternate models can complicate this picture (Knutti et al. 2010).

Model Validation. We define model validity in the context of "good" prediction of a given QOI. We will use one subset of the data for model calibration and inference of model plausibility, while other subsets will be used for establishing agreement with model predictions, hence validation. In this context, selection of which data to use for validation can be aided by fingerprint methods (Santer et al. 1996). Fingerprint methods have been used e.g., in the detection/attribution of the causes of global warming to match patterns of observed temperature change to patterns expected from combinations of various causes. We propose to generalize this methodology of pattern matching for model validation.

APPENDIX 5: ABBREVIATED TERMS

ABBREVIATED TERMS

1D	one-dimensional
2D	two-dimensional
3D	three-dimensional
ACRF	ARM Climate Research Facility
AD	automatic differentiation
AERI	Atmospheric Emitted Radiance InterfErometer
AIC	Akaike information criterion
AIRS	Atmospheric Infrared Sounder
ALCF	Argonne Leadership Computing Facility
AMD	Advanced Micro Devices
AMF	ARM Mobile Facility
AMR	Adaptive Mesh Refinement
AMSR-E	Advanced Microwave Scanning Radiometer for EOS
ANL	Argonne National Laboratory
AOGCM	Atmospheric and Oceanic General Circulation Model
AOMIP	Arctic Ocean Model Intercomparison Project
APDEC	Applied Partial Differential Equations Center
APE	aqua-planet
API	application progam interface
AR4	IPCC Fourth Assessment Report
ARM	Atmospheric Research Measurement
ASC	Advanced Simulation and Computing
ASD	Atmospheric Sciences Division
ASR	Atmospheric System Research
BE	broadband engine
BER	DOE Office of Biological and Environmental Research
BIC	Bayesian information criterion
BMA	Bayesian Model Averaging
BNL	Brookhaven National Laboratory
BOREAS	Boreal Ecosystem Atomosphere Study
CAM	Community Atmosphere Model
CAPE	convective available potential energy

CAR	Computing Applications and Research
CASC	Center for Applied Scientific Computing
CCSM	Community Climate System Model
CDAT	Climate Data Analysis Tools
CDIAC	Carbon Dioxide Information Analysis Center
CERES	Clouds and Earth’s Radiant Energy System
CESM	Community Earth System Model
CET	Center for Enabling Technologies
CF	Climate and Forecast
CF	cloud fraction
CFAD	cloud frequency altitude diagram
CHAMMP	Computer Hardware, Advanced Mathematics and Model Physics
CI	component interface
C-LAMP	Carbon Land-Modeling Intercomparison Project
CLIVAR	Climate Variability and Predictability
CLM	Community Land Model
CLM-CN	CLM-Nitrogen Cycle
CMAP	Climate Prediction Center Merged Analysis of Precipitation
CMBE	Climate Modeling Best Estimate
CORE	Common Ocean Reference Experiment
CPL7	CESM Version 7 Coupler
CPU	central processing unit
CSML	Climate Science Modeling Language
CSRI	Computer Science Research Institute
CSRM	cloud-system resolving model
CSSEF	Climate Science for a Sustainable Energy Future
CUDA	Compute Unified Device Architecture
DAAC	Distributed Active Archive Center
DAKOTA	Design Analysis Kit for Optimization
DIT	Data Infrastructure and Test Bed
DOE	U.S. Department of Energy
EBIS	Enriched Background Isotope Study
ECMWF	European Centre for Medium-Range Weather Forecasts
ED	Ecosystem Demography
EDEN	Ensemble Data Analysis Environment

EIS	estimated inversion strength
eMI	e-Minerals Infrastructure
EMSL	Environmental Molecular Science Laboratory
EnKF	Ensemble Kalman Filter
EOS	Earth Observing System
ERA	ECMWF Re-Analysis
ERBE	Earth Radiation Budget Experiment
ERCAP	Energy Research Computing Allocations Process
ESG	Earth System Grid
ESG-CET	Earth System Grid Center for Enabling Technologies
ESM	Earth System Model
ESnet	Energy Sciences Network
ESRL	Earth System Research Laboratory
ET	evapotranspiration
EVP	elastic-viscous-plastic
EXACCT	Exascale Climate Co-design Team
FAB	Fixed Age Bin
FACE	Free Air CO_2 Enrichment
FIFE	First International Satellite Land Surface Climatology Project) Field Experiment
FPAR	fraction of absorbed photosynthetically active radiation
FTE	full-time equivalent
FV-AMR	finite-volume adaptive mesh refinement
FWP	field work proposal
GASP	Global Atmospheric Sampling Program
GB	gigabyte
Gbit	gigabit
Gbps	gigabit per second
GCAM	Global Change Analysis Model
GCM	General Circulation Model
GDAL	Geospatial Data Abstraction Library
GDO	Green Data Oasis
GDO2	Green Data Oasis 2
GHCND	Global Historical Climate Network–Daily
GHG	greenhouse gas
GIS	Geographic Information System

GLODAP	Global Ocean Data Analysis Project
GM	Gent-McWilliams
GMD	Global Monitoring Division
GO-ESSP	Global Organization for Earth System Science Portals
GP	Gaussian Process
GPCP	Global Precipitation Climatology Project
GPP	Gross Primary Productivity
GPS	Global Positioning System
GPU	graphics processing unit
GRACE	Gravity Recovery and Climate Experiment
HadISST	Hadley Centre Sea Ice and Sea Surface Temperature Data Set
HDF	Hierarchical Data Format
HDMR	High Dimensional Model Representation
HIRS	High-Resolution Infrared Radiation Sounder
HOMME	High-Order Method Modeling Environment
HPC	high-performance computing
HPSS	High-Performance Storage System
HRR	Hillslope River Routing
HYPOP	Hybrid Coordinate Parallel Ocean Program
I/O	Input/Output
IB	InfiniBand
IBTrACs	International Best Track Archive for Climate Stewardship
ICOADS	International Comprehensive Ocean-Atmosphere Data Set
IMPACTS	Investigation of the Magnitudes and Probabilities of Abrupt Climate Transitions
INCITE	Innovative and Novel Computational Impact on Theory and Experiment
INTERFACE	Integrated Network for Terrestrial Ecosystem Research on Feedbacks to the Atmosphere and Climate
IP	input parameter
IPCC	Intergovernmental Panel on Climate Change
ISCCP	International Satellite Cloud Climatology Project
ISDE	Integrated Software Development Environment
ISICLES	Ice Sheet Initiative for Climate Extremes
JFNK	Jacobian-Free Newton-Krylov
JGCRI	Joint Global Change Research Institute
KL	Karhunen-Loeve

KPCA	kernel principal component analysis
LAI	leaf area index
LANL	Los Alamos National Laboratory
LANS	Lagrangian-Averaged Navier Stokes
LBNL	Lawrence Berkeley National Laboratory
LC	Livermore Computing
LCF	Leadership Computing Facility
LDAS	Land Data Assimilation System
LES	large-eddy simulation
LHS	Latin Hypercube Sampling
LLNL	Lawrence Livermore National Laboratory
LTER	Long-Term Ecological Research
LTM	long-term measure
LTS	lower troposphere stability
LTS	lower tropospheric stability
LW	long wave
LWP	liquid water path
MAOC	mineral-associated organic carbon
MARS	Multivariate Adaptive Regression Splines
MAST-DC	Modeling and Synthesis Thematic Data Center
mb	millibar
MCMC	Markov chain Monte Carlo
MCT	Model Coupling Toolkit
METAFOR	Metadata for Climate Modeling Digital Repositories
MJO	Madden-Julian Oscillation
ML	maximum likelihood
MMM	Mesoscale and Microscale Meteorology
MOAB	Mesh-Oriented datABase
MOAT	Morris one-at-a-time
MODIS	Moderate Resolution Imaging Spectroradiometer
MOZAIC	Measurements of Ozone, Water Vapour, Carbon Monoxide, and Nitrogen Oxides by in-service Arbus Aircraft
MPAS	Model for Prediction Across Scales
MPAS-O	MPAS Ocean Model
MPI	message-passing interface

MSS	mass storage system
NACP	North American Carbon Program
NASA	National Aeronautics and Space Administration
NCAR	National Center for Atmospheric Research
NCEP	National Centers for Environmental Prediction
NCL	National Center for Atmospheric Research Command Language
NEAMS	Nuclear Energy Advanced Modeling and Simulation
NERC	Natural Environment Research Council
NERSC	National Energy Research Scientific Computing Center
NetCDF	Network Common Data Format
NEWS	NASA Energy and Water Cycle
NOAA	National Oceanic and Atmospheric Administration
NSF	National Science Foundation
NSIDC	National Snow and Ice Data Center
OGC	Open Geospatial Consortium
OGR	GDAL Open-Source Geospatial Library
OLCF	ORNL Leadership Computing Facility
OpenCL	Open Computing Language
ORNL	Oak Ridge National Laboratory
ParMETIS	Parallel Graph Partitioning and Sparse Matrix Ordering Library
PB	petabyte
PCA	principal component analysis
PCE	polynomial chaos expansion
PCMDI	Program for Climate Model Diagnosis and Intercomparison
PDE	partial differential equation
PDF	probability distribution function
PF	petaflop
PFT	plant functional type
PGD	Proper Generalized Decomposition
PHC	Polar Science Center Hydrographic Climatology
PI	principal investigator
PMC	Path-Integral Monte Carlo
PNNL	Pacific Northwest National Laboratory
POP	Parallel Ocean Program
PRECIP	precipitation rate

PV	parallel vorticity
PWV	precipitable water vapor
Q/SQ	quadrature/sparse-quadrature
QDR	quad data rate
QOI	quantity of interest
RAID	redundant array of independent disks
RAM	random access memory
RCN	Research Coordination Network
REOS	Repository for Evaluating Ocean Simulations
RH	relative humidity
RIPBE	Radiatively Important Parameters Best Estimate
RTM	river transport model
SA	sensitivity analysis
SAN	storage area network
SC	DOE Office of Science
SciDAC	Scientific Discovery through Advanced Computing
SCRIP	Spherical Coordinate Remapping and Interpolation Package
SEAM	Spectral Element Atmosphere Model
SGP	ARM Southern Great Plains Site
SMC	Simulation Monte Carlo
SMP	symmetric multiprocessor
SNL	Sandia National Laboratories
SOM	soil organic matter
SPMD	single-process, multiple data
SSM	special sensor microwave
SST	Sea Surface Temperature
SSU	Storage Scalable Unit
SW	short wave
SWE	shallow water equation
SYPD	simulated years per day
T	temperature
TB	terabyte
TDI	Testbed and Data Infrastructure
TF	teraflop (10^{12} floating point operations per second)
THC	thermohaline circulation

TRMM	Tropical Rainfall Measuring Mission
UK NERC	UK Natural Environmental Research Council
UQ	Uncertainty Quantification
USFS	U.S. Forest Service
USGS	United States Geological Survey
UTC	Coordinated Universal Time
UV-CDAT	Ultra-Scale Visualization Climate Data Analysis Tools
VBD	variance-based decomposition
WMO	World Meteorological Organization
WRF	Weather Research and Forecasting Model